

APBS

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Chapter 1

APBS Programmers Guide

APBS was written by Nathan A. Baker.
Additional contributing authors listed in the code documentation.

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1.2 License

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This documentation provides information about the programming interface provided by the APBS software and a general guide to linking to the APBS libraries. Information about installation, configuration, and general usage can be found in the [User's Guide](#).

1.3 Programming Style

APBS was developed following the [Clean OO C](#) style of Mike Holst. In short, Clean OO C code is written in a object-oriented, ISO C-compliant fashion, and can be compiled with either a C or C++ compiler.

Following this formalism, all public data is enclosed in structures which resemble C++ classes. These structures and member functions are then declared in a public header file which provides a concise description of the interface for the class. Private functions and data are included in private header files (or simply the source code files themselves) which are not distributed. When using the library, the end-user only sees the public header file and the compiled library and is therefore (hopefully) oblivious to the private members and functions. Each class is also equipped with a constructor and destructor function which is responsible for allocating and freeing any memory required by the instantiated objects. As mentioned above, public data members are enclosed in C structures which are visible to the end-user. Public member functions are generated by mangling the class and function names *and* passing a pointer to the object on which the member function is supposed to act. For example, a public member function with the C++ declaration

```
public double Foo::bar(int i, double d)
```

would be declared as

```
VEXTERNC double Foo_bar(Foo *thee, int i, double d)
```

where `VEXTERNC` is a compiler-dependent macro, the underscore `_` replaces the C++ double-colon `::`, and `thee` replaces the `this` variable implicit in all C++ classes. Since they do not appear in public header files, private functions could be declared in any format pleasing to the user, however, the above declaration convention should generally be used for both public and private functions. Within the source code, the public and private function declarations/definitions are prefaced by the macros `VPUBLIC` and `VPRIVATE`, respectively. These are macros which reduce global name pollution, similar to encapsulating private data within C++ classes.

The only C++ functions not explicitly covered by the above declaration scheme are the constructors (used to allocate and initialize class data members) and destructors (used to free allocated memory). These are declared in the following fashion: a constructor with the C++ declaration

```
public void Foo::Foo(int i, double d)
```

would be declared as

```
VEXTERNC Foo* Foo_ctor(int i, double d)
```

which returns a pointer to the newly constructed `Foo` object. Likewise, a destructor declared as

```
public void Foo::~~Foo()
```

in C++ would be

```
VEXTERNC void Foo_dtor(Foo **thee)
```

in Clean OO C.

Finally, inline functions in C++ are simply treated as macros in Clean OO C and declared/defined using `define` statements in the public header file.

See any of the APBS header files for more information on Clean OO C programming styles.

1.4 Application programming interface documentation

The API documentation for this code was generated by [doxygen](#). You can either view the API documentation by using the links at the top of this page, or the slight re-worded/re-interpreted list below:

- [Class overview](#)
- [Class declarations](#)
- [Class members](#)
- [Class methods](#)

Chapter 2

Bug List

Global **Bmat_printHB** (Bmat *thee, char *fname)

Hardwired to only handle the single block symmetric case.

Global **energyFE** (NOsh *nosh, int icalc, Vfetk *fetk[NOSH_MAXCALC], int *nenergy, double *totEnergy, double *qfEnergy, double *qmEnergy, double *dielEnergy)

"calcenergy 2" does not work

Global **initFE** (int icalc, NOsh *nosh, FEMparm *feparm, PBEparm *pbeparm, Vpbe *pbe[NOSH_MAXCALC], Valist *alist[NOSH_MAXMOL], Vfetk *fetk[NOSH_MAXCALC])

THIS FUNCTION IS HARD-CODED TO SOLVE LRPBE

THIS FUNCTION IS HARD-CODED TO SOLVE LRPBE

Struct **sVpmgp**

Value ipcon does not currently allow for preconditioning in PMG

Global **Vacc_fastMolAcc** (Vacc *thee, double center[VAPBS_DIM], double radius)

This routine has a slight bug which can generate very small internal regions of high dielectric (thanks to John Mongan and Jess Swanson for finding this)

Global **Vacc_molAcc** (Vacc *thee, double center[VAPBS_DIM], double radius)

This routine has a slight bug which can generate very small internal regions of high dielectric (thanks to John Mongan and Jess Swanson for finding this)

Global **Vfetk_dumpLocalVar** ()

This function is not thread-safe

Global **Vfetk_externalUpdateFunction** (SS **simps, int num)

This function is not thread-safe.

Global **Vfetk_fillArray** (Vfetk *thee, Bvec *vec, Vdata_Type type)

Several values of type are not implemented

Global **Vfetk_PDE_ctor** (Vfetk *fetk)

Not thread-safe

Global **Vfetk_PDE_ctor2** (PDE *thee, Vfetk *fetk)

Not thread-safe

Global **Vfetk_PDE_delta** (PDE *thee, int type, int chart, double txq[], void *user, double F[])

This function is not thread-safe

Global **Vfetk_PDE_DFu_wv** (PDE *thee, int key, double W[], double dW[][VAPBS_DIM], double V[], double dV[][VAPBS_DIM])

This function is not thread-safe

Global **Vfetk_PDE_Fu** (PDE *thee, int key, double F[])

This function is not thread-safe

This function is not implemented (sets error to zero)

Global **Vfetk_PDE_Fu_v** (PDE *thee, int key, double V[], double dV[][VAPBS_DIM])

This function is not thread-safe

Global **Vfetk_PDE_initElement** (PDE *thee, int elementType, int chart, double tvx[][VAPBS_DIM], void *data)

This function is not thread-safe

Global **Vfetk_PDE_initFace** (PDE *thee, int faceType, int chart, double tvec[])

This function is not thread-safe

Global **Vfetk_PDE_initPoint** (PDE *thee, int pointType, int chart, double txq[], double tU[], double tdU[][VAPBS_DIM])

This function is not thread-safe

This function uses pre-defined boundary definitions for the molecular surface.

Global **Vfetk_PDE_Ju** (PDE *thee, int key)

This function is not thread-safe.

Global **Vfetk_PDE_markSimplex** (int dim, int dimll, int simplexType, int faceType[VAPBS_NVS], int vertexType[VAPBS_NVS], int chart[], double vx[][VAPBS_DIM], void *simplex)

This function is not thread-safe

Global **Vfetk_PDE_u_D** (PDE *thee, int type, int chart, double txq[], double F[])

This function is hard-coded to call only multiple-sphere Debye-Hückel functions.

This function is not thread-safe.

Global **Vfetk_PDE_u_T** (PDE *thee, int type, int chart, double txq[], double F[])

This function is not thread-safe.

Global **Vfetk_write** (Vfetk *thee, const char *iodev, const char *iofmt, const char *thost, const char *fname, Bvec *vec, Vdata_Format format)

Some values of format are not implemented

Global **Vgreen_helmholtz** (Vgreen *thee, int npos, double *x, double *y, double *z, double *val, double kappa)

Not implemented yet

Global **Vgreen_helmholtzD** (Vgreen *thee, int npos, double *x, double *y, double *z, double *gradx, double *grady, double *gradz, double kappa)

Not implemented yet

Global **Vgrid_writeUHBD** (Vgrid *thee, const char *iodev, const char *iofmt, const char *thost, const char *fname, char *title, double *pvec)

This routine does not respect partition information

Global **Vpackmg** (int *iparm, double *rparm, size_t *nrwk, int *niwk, int *nx, int *ny, int *nz, int *nlev, int *nu1, int *nu2, int *mgkey, int *itmax, int *istop, int *ipcon, int *nonlin, int *mgsmoo, int *mgprol, int *mgcoar, int *mgsolv, int *mgdisc, int *iinfo, double *errtol, int *ipkey, double *omegal, double *omegan, int *irite, int *iperf)

Can this path variable be replaced with a Vio socket?

Global **Vpbe_ctor2** (Vpbe *thee, Valist *alist, int ionNum, double *ionConc, double *ionRadii, double *ionQ, double T, double soluteDiel, double solventDiel, double solventRadius, int focusFlag, double sdens, double z_mem, double L, double membraneDiel, double V)

The focusing flag is currently not used!!

Global **Vpee_markRefine** (Vpee *thee, AM *am, int level, int akey, int rcol, double etol, int bkey)

This function is no longer up-to-date with FEtk and may not function properly

Global **Vpmg_fillco** (Vpmg *thee, Vsurf_Meth surfMeth, double splineWin, Vchrg_Meth chargeMeth, int useDielXMap, Vgrid *dielXMap, int useDielYMap, Vgrid *dielYMap, int useDielZMap, Vgrid *dielZMap, int useKappaMap, Vgrid *kappaMap, int usePotMap, Vgrid *potMap, int useChargeMap, Vgrid *chargeMap)

useDielMap could only be passed once, not three times, to this function - why not just once? that's what the call in [routines.c](#) ends up doing - just passing useDielMap three times. - P. Ellis 11/3/11

Global **Vpmg_printColComp** (Vpmg *thee, char path[72], char title[72], char mxtype[3], int flag)

Can this path variable be replaced with a Vio socket?

Chapter 3

Deprecated List

Global [sMGparm::nlev](#)

Just ignored now

Chapter 4

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Chapter 7

Topic Documentation

7.1 dependencies

7.2 Vcsm class

A charge-simplex map for evaluating integrals of delta functions in a finite element setting.

Files

- file [vcsm.c](#)
Class Vcsm methods.
- file [vcsm.h](#)
Contains declarations for the Vcsm class.

Data Structures

- struct [sVcsm](#)
Charge-simplex map class.

Typedefs

- typedef struct [sVcsm](#) [Vcsm](#)
Declaration of the Vcsm class as the Vcsm structure.

Functions

- VEXTERNC void [Gem_setExternalUpdateFunction](#) ([Gem](#) *thee, void(*externalUpdate)(SS **simps, int num))
External function for FEtk Gem class to use during mesh refinement.
- VEXTERNC [Valist](#) * [Vcsm_getValist](#) ([Vcsm](#) *thee)
Get atom list.
- VEXTERNC int [Vcsm_getNumberAtoms](#) ([Vcsm](#) *thee, int isimp)
Get number of atoms associated with a simplex.
- VEXTERNC [Vatom](#) * [Vcsm_getAtom](#) ([Vcsm](#) *thee, int iatom, int isimp)
Get particular atom associated with a simplex.
- VEXTERNC int [Vcsm_getAtomIndex](#) ([Vcsm](#) *thee, int iatom, int isimp)
Get ID of particular atom in a simplex.
- VEXTERNC int [Vcsm_getNumberSimplices](#) ([Vcsm](#) *thee, int iatom)

Get number of simplices associated with an atom.

- VEXTERNC SS * [Vcsm_getSimplex](#) ([Vcsm](#) *thee, int isimp, int iatom)

Get particular simplex associated with an atom.

- VEXTERNC int [Vcsm_getSimplexIndex](#) ([Vcsm](#) *thee, int isimp, int iatom)

Get index particular simplex associated with an atom.

- VEXTERNC unsigned long int [Vcsm_memChk](#) ([Vcsm](#) *thee)

Return the memory used by this structure (and its contents) in bytes.

- VEXTERNC [Vcsm](#) * [Vcsm_ctor](#) ([Valist](#) *alist, [Gem](#) *gm)

Construct Vcsm object.

- VEXTERNC int [Vcsm_ctor2](#) ([Vcsm](#) *thee, [Valist](#) *alist, [Gem](#) *gm)

FORTTRAN stub to construct Vcsm object.

- VEXTERNC void [Vcsm_dtor](#) ([Vcsm](#) **thee)

Destroy Vcsm object.

- VEXTERNC void [Vcsm_dtor2](#) ([Vcsm](#) *thee)

FORTTRAN stub to destroy Vcsm object.

- VEXTERNC void [Vcsm_init](#) ([Vcsm](#) *thee)

Initialize charge-simplex map with mesh and atom data.

- VEXTERNC int [Vcsm_update](#) ([Vcsm](#) *thee, SS **simps, int num)

Update the charge-simplex and simplex-charge maps after refinement.

7.2.1 Detailed Description

A charge-simplex map for evaluating integrals of delta functions in a finite element setting.

7.2.2 Typedef Documentation

7.2.2.1 Vcsm

```
typedef struct sVcsm Vcsm
```

Declaration of the Vcsm class as the Vcsm structure.

Definition at line 122 of file [vcsm.h](#).

7.2.3 Function Documentation

7.2.3.1 Gem_setExternalUpdateFunction()

```
VEXTERNC void Gem_setExternalUpdateFunction (
    Gem * thee,
    void(*) (SS **simps, int num) externalUpdate )
```

External function for FEtk Gem class to use during mesh refinement.

Author

Nathan Baker

Parameters

<i>thee</i>	The FEtk geometry manager
<i>externalUpdate</i>	Function pointer for call during mesh refinement

7.2.3.2 Vcsm_ctor()

```

VEXTERNC Vcsm * Vcsm_ctor (
    Valist * alist,
    Gem * gm )

```

Construct Vcsm object.

Author

Nathan Baker

Note

- The initial mesh must be sufficiently coarse for the assignment procedures to be efficient
- The map is not built until Vcsm_init is called

Returns

Pointer to newly allocated Vcsm object

Parameters

<i>alist</i>	List of atoms
<i>gm</i>	FEtk geometry manager defining the mesh

Definition at line 136 of file [vcsm.c](#).

7.2.3.3 Vcsm_ctor2()

```

VEXTERNC int Vcsm_ctor2 (
    Vcsm * thee,
    Valist * alist,
    Gem * gm )

```

FORTTRAN stub to construct Vcsm object.

Author

Nathan Baker

Note

- The initial mesh must be sufficiently coarse for the assignment procedures to be efficient
- The map is not built until Vcsm_init is called

Returns

1 if successful, 0 otherwise

Parameters

<i>thee</i>	The Vcsm object
<i>alist</i>	The list of atoms
<i>gm</i>	The FEtk geometry manager defining the mesh

Definition at line 147 of file [vcsn.c](#).

7.2.3.4 Vcsn_dtor()

```
VEXTERNC void Vcsn_dtor (
    Vcsn ** thee )
```

Destroy Vcsn object.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to memory location for Vcsn object
-------------	--

Definition at line 292 of file [vcsn.c](#).

7.2.3.5 Vcsn_dtor2()

```
VEXTERNC void Vcsn_dtor2 (
    Vcsn * thee )
```

FORTTRAN stub to destroy Vcsn object.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to Vcsn object
-------------	------------------------

Definition at line 300 of file [vcsn.c](#).

7.2.3.6 Vcsn_getAtom()

```
VEXTERNC Vatom * Vcsn_getAtom (
    Vcsn * thee,
    int iatom,
    int isimp )
```

Get particular atom associated with a simplex.

Author

Nathan Baker

Returns

Array of atoms associated with a simplex

Parameters

<i>thee</i>	The Vcsn object
<i>iatom</i>	Index of atom in Vcsn list ofr this simplex
<i>isimp</i>	Simplex ID

Definition at line 77 of file [vcsm.c](#).

7.2.3.7 Vcsm_getAtomIndex()

```
VEXTERNC int Vcsm_getAtomIndex (
    Vcsm * thee,
    int iatom,
    int isimp )
```

Get ID of particular atom in a simplex.

Author

Nathan Baker

Returns

Index of atom in Valist object

Parameters

<i>thee</i>	The Vcsm object
<i>iatom</i>	Index of atom in Vcsm list for this simplex
<i>isimp</i>	Simplex ID

Definition at line 88 of file [vcsm.c](#).

7.2.3.8 Vcsm_getNumberAtoms()

```
VEXTERNC int Vcsm_getNumberAtoms (
    Vcsm * thee,
    int isimp )
```

Get number of atoms associated with a simplex.

Author

Nathan Baker

Returns

Number of atoms associated with a simplex

Parameters

<i>thee</i>	The Vcsm object
<i>isimp</i>	Simplex ID

Definition at line 69 of file [vcsm.c](#).

7.2.3.9 Vcsm_getNumberSimplices()

```
VEXTERNC int Vcsm_getNumberSimplices (
    Vcsm * thee,
    int iatom )
```

Get number of simplices associated with an atom.

Author

Nathan Baker

Returns

Number of simplices associated with an atom

Parameters

<i>thee</i>	The Vcsm object
<i>iatom</i>	The Valist atom index

Definition at line 99 of file [vcsm.c](#).**7.2.3.10 Vcsm_getSimplex()**

```
VEXTERNC SS * Vcsm_getSimplex (
    Vcsm * thee,
    int isimp,
    int iatom )
```

Get particular simplex associated with an atom.

Author

Nathan Baker

Returns

Pointer to simplex object

Parameters

<i>thee</i>	The Vcsm object
<i>isimp</i>	Index of simplex in Vcsm list
<i>iatom</i>	Valist atom index

Definition at line 109 of file [vcsm.c](#).**7.2.3.11 Vcsm_getSimplexIndex()**

```
VEXTERNC int Vcsm_getSimplexIndex (
    Vcsm * thee,
    int isimp,
    int iatom )
```

Get index particular simplex associated with an atom.

Author

Nathan Baker

Returns

Gem index of specified simplex

Parameters

<i>thee</i>	The Vcsm object
<i>isimp</i>	Index of simplex in Vcsm list
<i>iatom</i>	Index of atom in Valist

Definition at line 119 of file [vcsm.c](#).

7.2.3.12 Vcsm_getValist()

```
VEXTERNC Valist * Vcsm_getValist (
    Vcsm * thee )
```

Get atom list.

Author

Nathan Baker

Returns

Pointer to Valist atom list

Parameters

<i>thee</i>	The Vcsm object
-------------	-----------------

Definition at line 62 of file [vcsm.c](#).

7.2.3.13 Vcsm_init()

```
VEXTERNC void Vcsm_init (
    Vcsm * thee )
```

Initialize charge-simplex map with mesh and atom data.

Author

Nathan Baker

Note

The initial mesh must be sufficiently coarse for the assignment procedures to be efficient

Parameters

<i>thee</i>	The Vcsm object
-------------	-----------------

Definition at line 170 of file [vcsm.c](#).

7.2.3.14 Vcsm_memChk()

```
VEXTERNC unsigned long int Vcsm_memChk (
    Vcsm * thee )
```

Return the memory used by this structure (and its contents) in bytes.

Author

Nathan Baker

Returns

The memory used by this structure and its contents in bytes

Parameters

<i>thee</i>	The Vcsm object
-------------	-----------------

Definition at line 129 of file [vcsm.c](#).**7.2.3.15 Vcsm_update()**

```

VEXTERNC int Vcsm_update (
    Vcsm * thee,
    SS ** simps,
    int num )

```

Update the charge-simplex and simplex-charge maps after refinement.

Author

Nathan Baker

Returns

1 if successful, 0 otherwise

Parameters

<i>thee</i>	The Vcsm object
<i>simps</i>	List of pointer to newly created (by refinement) simplex objects. The first simplex is expected to be derived from the parent simplex and therefore have the same ID. The remaining simplices are the children and should represent new entries in the charge-simplex map.
<i>num</i>	Number of simplices in simps list

Definition at line 326 of file [vcsm.c](#).**7.3 Vfetk class**

FEtk master class (interface between FEtk and APBS)

Files

- file [vfetk.c](#)
Class Vfetk methods.
- file [vfetk.h](#)
Contains declarations for class Vfetk.

Data Structures

- struct `sVfetk`
Contains public data members for Vfetk class/module.
- struct `sVfetk_LocalVar`
Vfetk LocalVar subclass.

Macros

- `#define VRINGMAX 1000`
Maximum number of simplices in a simplex ring.
- `#define VATOMMAX 1000000`
Maximum number of atoms associated with a vertex.

Typedefs

- typedef enum `eVfetk_LsolvType` `Vfetk_LsolvType`
Declare FEMparm_LsolvType type.
- typedef enum `eVfetk_MeshLoad` `Vfetk_MeshLoad`
Declare FEMparm_GuessType type.
- typedef enum `eVfetk_NsolvType` `Vfetk_NsolvType`
Declare FEMparm_NsolvType type.
- typedef enum `eVfetk_GuessType` `Vfetk_GuessType`
Declare FEMparm_GuessType type.
- typedef enum `eVfetk_PrecType` `Vfetk_PrecType`
Declare FEMparm_GuessType type.
- typedef struct `sVfetk_LocalVar` `Vfetk_LocalVar`
Declaration of the Vfetk_LocalVar subclass as the Vfetk_LocalVar structure.

Enumerations

- enum `eVfetk_LsolvType` { `VLT_SLU` =0 , `VLT_MG` =1 , `VLT_CG` =2 , `VLT_BCG` =3 }
Linear solver type.
- enum `eVfetk_MeshLoad` { `VML_DIRICUBE` , `VML_NEUMCUBE` , `VML_EXTERNAL` }
Mesh loading operation.
- enum `eVfetk_NsolvType` { `VNT_NEW` =0 , `VNT_INC` =1 , `VNT_ARC` =2 }
Non-linear solver type.
- enum `eVfetk_GuessType` { `VGT_ZERO` =0 , `VGT_DIRI` =1 , `VGT_PREV` =2 }
Initial guess type.
- enum `eVfetk_PrecType` { `VPT_IDEN` =0 , `VPT_DIAG` =1 , `VPT_MG` =2 }
Preconditioner type.

Functions

- `VPUBLIC double Vfetk_energy (Vfetk *thee, int color, int nonlin)`
Return the total electrostatic energy.
- `VEXTERNNC Gem * Vfetk_getGem (Vfetk *thee)`
Get a pointer to the Gem (grid manager) object.
- `VEXTERNNC AM * Vfetk_getAM (Vfetk *thee)`
Get a pointer to the AM (algebra manager) object.

- VEXTERNC [Vpbe](#) * [Vfetk_getVpbe](#) ([Vfetk](#) *thee)
Get a pointer to the Vpbe (PBE manager) object.
- VEXTERNC [Vcsm](#) * [Vfetk_getVcsm](#) ([Vfetk](#) *thee)
Get a pointer to the Vcsm (charge-simplex map) object.
- VEXTERNC int [Vfetk_getAtomColor](#) ([Vfetk](#) *thee, int iatom)
Get the partition information for a particular atom.
- VEXTERNC [Vfetk](#) * [Vfetk_ctor](#) ([Vpbe](#) *pbe, [Vhal_PBEType](#) type)
Constructor for Vfetk object.
- VEXTERNC int [Vfetk_ctor2](#) ([Vfetk](#) *thee, [Vpbe](#) *pbe, [Vhal_PBEType](#) type)
FORTTRAN stub constructor for Vfetk object.
- VEXTERNC void [Vfetk_dtor](#) ([Vfetk](#) **thee)
Object destructor.
- VEXTERNC void [Vfetk_dtor2](#) ([Vfetk](#) *thee)
FORTTRAN stub object destructor.
- VEXTERNC double * [Vfetk_getSolution](#) ([Vfetk](#) *thee, int *length)
Create an array containing the solution (electrostatic potential in units of $k_B T/e$) at the finest mesh level.
- VEXTERNC void [Vfetk_setParameters](#) ([Vfetk](#) *thee, [PBEparm](#) *pbeparm, [FEMparm](#) *feparm)
Set the parameter objects.
- VEXTERNC double [Vfetk_dqmEnergy](#) ([Vfetk](#) *thee, int color)
Get the "mobile charge" and "polarization" contributions to the electrostatic energy.
- VEXTERNC double [Vfetk_qfEnergy](#) ([Vfetk](#) *thee, int color)
Get the "fixed charge" contribution to the electrostatic energy.
- VEXTERNC unsigned long int [Vfetk_memChk](#) ([Vfetk](#) *thee)
Return the memory used by this structure (and its contents) in bytes.
- VEXTERNC void [Vfetk_setAtomColors](#) ([Vfetk](#) *thee)
Transfer color (partition ID) information frmo a partitioned mesh to the atoms.
- VEXTERNC void [Bmat_printHB](#) ([Bmat](#) *thee, char *fname)
Writes a Bmat to disk in Harwell-Boeing sparse matrix format.
- VEXTERNC [Vrc_Codes](#) [Vfetk_genCube](#) ([Vfetk](#) *thee, double center[3], double length[3], [Vfetk_MeshLoad](#) meshType)
Construct a rectangular mesh (in the current Vfetk object)
- VEXTERNC [Vrc_Codes](#) [Vfetk_loadMesh](#) ([Vfetk](#) *thee, double center[3], double length[3], [Vfetk_MeshLoad](#) meshType, [Vio](#) *sock)
Loads a mesh into the Vfetk (and associated) object(s).
- VEXTERNC [PDE](#) * [Vfetk_PDE_ctor](#) ([Vfetk](#) *fetk)
Constructs the FEtk PDE object.
- VEXTERNC int [Vfetk_PDE_ctor2](#) ([PDE](#) *thee, [Vfetk](#) *fetk)
Intializes the FEtk PDE object.
- VEXTERNC void [Vfetk_PDE_dtor](#) ([PDE](#) **thee)
Destroys FEtk PDE object.
- VEXTERNC void [Vfetk_PDE_dtor2](#) ([PDE](#) *thee)
FORTTRAN stub: destroys FEtk PDE object.
- VEXTERNC void [Vfetk_PDE_initAssemble](#) ([PDE](#) *thee, int ip[], double rp[])
Do once-per-assembly initialization.
- VEXTERNC void [Vfetk_PDE_initElement](#) ([PDE](#) *thee, int elementType, int chart, double txx[][[VAPBS_DIM](#)], void *data)
Do once-per-element initialization.

- VEXTERNC void `Vfetk_PDE_initFace` (PDE *thee, int faceType, int chart, double tvec[])
Do once-per-face initialization.
- VEXTERNC void `Vfetk_PDE_initPoint` (PDE *thee, int pointType, int chart, double txq[], double tU[], double tdU[][VAPBS_DIM])
Do once-per-point initialization.
- VEXTERNC void `Vfetk_PDE_Fu` (PDE *thee, int key, double F[])
Evaluate strong form of PBE. For interior points, this is:
- VEXTERNC double `Vfetk_PDE_Fu_v` (PDE *thee, int key, double V[], double dV[][VAPBS_DIM])
This is the weak form of the PBE; i.e. the strong form integrated with a test function to give:
- VEXTERNC double `Vfetk_PDE_DFu_wv` (PDE *thee, int key, double W[], double dW[][VAPBS_DIM], double V[], double dV[][VAPBS_DIM])
This is the linearization of the weak form of the PBE; e.g., for use in a Newton iteration. This is the functional linearization of the strong form integrated with a test function to give:
- VEXTERNC void `Vfetk_PDE_delta` (PDE *thee, int type, int chart, double txq[], void *user, double F[])
Evaluate a (discretized) delta function source term at the given point.
- VEXTERNC void `Vfetk_PDE_u_D` (PDE *thee, int type, int chart, double txq[], double F[])
Evaluate the Dirichlet boundary condition at the given point.
- VEXTERNC void `Vfetk_PDE_u_T` (PDE *thee, int type, int chart, double txq[], double F[])
Evaluate the "true solution" at the given point for comparison with the numerical solution.
- VEXTERNC void `Vfetk_PDE_bisectEdge` (int dim, int dimII, int edgeType, int chart[], double vx[][VAPBS_DIM])
Define the way manifold edges are bisected.
- VEXTERNC void `Vfetk_PDE_mapBoundary` (int dim, int dimII, int vertexType, int chart, double vx[VAPBS_DIM])
Map a boundary point to some pre-defined shape.
- VEXTERNC int `Vfetk_PDE_markSimplex` (int dim, int dimII, int simplexType, int faceType[VAPBS_NVS], int vertexType[VAPBS_NVS], int chart[], double vx[][VAPBS_DIM], void *simplex)
User-defined error estimator – in our case, a geometry-based refinement method; forcing simplex refinement at the dielectric boundary and (for non-regularized PBE) the charges.
- VEXTERNC void `Vfetk_PDE_oneChart` (int dim, int dimII, int objType, int chart[], double vx[][VAPBS_DIM], int dimV)
Unify the chart for different coordinate systems – a no-op for us.
- VEXTERNC double `Vfetk_PDE_Ju` (PDE *thee, int key)
Energy functional. This returns the energy (less delta function terms) in the form:
- VEXTERNC void `Vfetk_externalUpdateFunction` (SS **simps, int num)
External hook to simplex subdivision routines in Gem. Called each time a simplex is subdivided (we use it to update the charge-simplex map)
- VEXTERNC int `Vfetk_PDE_simplexBasisInit` (int key, int dim, int comp, int *ndof, int dof[])
Initialize the bases for the trial or the test space, for a particular component of the system, at all quadrature points on the master simplex element.
- VEXTERNC void `Vfetk_PDE_simplexBasisForm` (int key, int dim, int comp, int pdkey, double xq[], double basis[])
Evaluate the bases for the trial or test space, for a particular component of the system, at all quadrature points on the master simplex element.
- VEXTERNC void `Vfetk_readMesh` (Vfetk *thee, int skey, Vio *sock)
Read in mesh and initialize associated internal structures.
- VEXTERNC void `Vfetk_dumpLocalVar` ()
Debugging routine to print out local variables used by PDE object.
- VEXTERNC int `Vfetk_fillArray` (Vfetk *thee, Bvec *vec, Vdata_Type type)
Fill an array with the specified data.
- VEXTERNC int `Vfetk_write` (Vfetk *thee, const char *iodev, const char *iofmt, const char *thost, const char *fname, Bvec *vec, Vdata_Format format)

Write out data.

- VEXTERNC Vrc_Codes [Vfetk_loadGem](#) ([Vfetk](#) *thee, Gem *gm)

Load a Gem geometry manager object into Vfetk.

7.3.1 Detailed Description

FEtk master class (interface between FEtk and APBS)

7.3.2 Macro Definition Documentation

7.3.2.1 VATOMMAX

```
#define VATOMMAX 1000000
```

Maximum number of atoms associated with a vertex.

Definition at line [1779](#) of file [vfetk.c](#).

7.3.2.2 VRINGMAX

```
#define VRINGMAX 1000
```

Maximum number of simplices in a simplex ring.

Definition at line [1776](#) of file [vfetk.c](#).

7.3.3 Typedef Documentation

7.3.3.1 Vfetk_GuessType

```
typedef enum eVfetk_GuessType Vfetk_GuessType
```

Declare FEMparm_GuessType type.

Definition at line [148](#) of file [vfetk.h](#).

7.3.3.2 Vfetk_LocalVar

```
typedef struct sVfetk_LocalVar Vfetk_LocalVar
```

Declaration of the Vfetk_LocalVar subclass as the Vfetk_LocalVar structure.

Definition at line [259](#) of file [vfetk.h](#).

7.3.3.3 Vfetk_LsolvType

```
typedef enum eVfetk_LsolvType Vfetk_LsolvType
```

Declare FEMparm_LsolvType type.

Definition at line [97](#) of file [vfetk.h](#).

7.3.3.4 Vfetk_MeshLoad

```
typedef enum eVfetk_MeshLoad Vfetk_MeshLoad
```

Declare FEMparm_GuessType type.

Definition at line [114](#) of file [vfetk.h](#).

7.3.3.5 Vfetk_NsolvType

```
typedef enum eVfetk_NsolvType Vfetk_NsolvType
```

Declare FEMparm_NsolvType type.

Definition at line [131](#) of file [vfetk.h](#).

7.3.3.6 Vfetk_PrecType

```
typedef enum eVfetk_PrecType Vfetk_PrecType
```

Declare FEMparm_GuessType type.

Definition at line 165 of file [vfetk.h](#).

7.3.4 Enumeration Type Documentation

7.3.4.1 eVfetk_GuessType

```
enum eVfetk_GuessType
```

Initial guess type.

Note

Do not change these values; they correspond to settings in FEtk

Enumerator

VGT_ZERO	Zero initial guess
VGT_DIRI	Dirichlet boundary condition initial guess
VGT_PREV	Previous level initial guess

Definition at line 138 of file [vfetk.h](#).

7.3.4.2 eVfetk_LsolvType

```
enum eVfetk_LsolvType
```

Linear solver type.

Note

Do not change these values; they correspond to settings in FEtk

Enumerator

VLT_SLU	SuperLU direct solve
VLT_MG	Multigrid
VLT_CG	Conjugate gradient
VLT_BCG	BiCGStab

Definition at line 86 of file [vfetk.h](#).

7.3.4.3 eVfetk_MeshLoad

```
enum eVfetk_MeshLoad
```

Mesh loading operation.

Enumerator

VML_DIRICUBE	Dirichlet cube
VML_NEUMCUBE	Neumann cube
VML_EXTERNAL	External mesh (from socket)

Definition at line 104 of file [vfetk.h](#).

7.3.4.4 eVfetk_NsolvType

enum [eVfetk_NsolvType](#)

Non-linear solver type.

Note

Do not change these values; they correspond to settings in FEtk

Enumerator

VNT_NEW	Newton solver
VNT_INC	Incremental
VNT_ARC	Psuedo-arclength

Definition at line 121 of file [vfetk.h](#).

7.3.4.5 eVfetk_PrecType

enum [eVfetk_PrecType](#)

Preconditioner type.

Note

Do not change these values; they correspond to settings in FEtk

Enumerator

VPT_IDEN	Identity matrix
VPT_DIAG	Diagonal scaling
VPT_MG	Multigrid

Definition at line 155 of file [vfetk.h](#).

7.3.5 Function Documentation

7.3.5.1 Bmat_printHB()

```

VEXTERNC void Bmat_printHB (
    Bmat * thee,
    char * fname )

```

Writes a Bmat to disk in Harwell-Boeing sparse matrix format.

Author

Stephen Bond

Note

This is a friend function of Bmat

Bug Hardwired to only handle the single block symmetric case.

Parameters

<i>thee</i>	The matrix to write
<i>fname</i>	Filename for output

Definition at line 1026 of file [vfetk.c](#).

7.3.5.2 Vfetk_ctor()

```

VEXTERNC Vfetk * Vfetk_ctor (
    Vpbe * pbe,
    Vhal_PBEType type )

```

Constructor for Vfetk object.

Author

Nathan Baker

Returns

Pointer to newly allocated Vfetk object

Note

This sets up the Gem, AM, and Aprx FEtk objects but does not create a mesh. The easiest way to create a mesh is to then call `Vfetk_genCube`

Parameters

<i>pbe</i>	Vpbe (PBE manager object)
<i>type</i>	Version of PBE to solve

Definition at line 532 of file [vfetk.c](#).

7.3.5.3 Vfetk_ctor2()

```

VEXTERNC int Vfetk_ctor2 (
    Vfetk * thee,
    Vpbe * pbe,
    Vhal_PBEType type )

```

FORTRAN stub constructor for Vfetk object.

Author

Nathan Baker

Returns

1 if successful, 0 otherwise

Note

This sets up the Gem, AM, and Aprx FEtk objects but does not create a mesh. The easiest way to create a mesh is to then call `Vfetk_genCube`

Parameters

<i>thee</i>	Vfetc object memory
<i>pbe</i>	PBE manager object
<i>type</i>	Version of PBE to solve

Definition at line 545 of file [vfetc.c](#).

7.3.5.4 Vfetc_dqmEnergy()

```
VEXTERNC double Vfetc_dqmEnergy (
    Vfetc * thee,
    int color )
```

Get the "mobile charge" and "polarization" contributions to the electrostatic energy.

Using the solution at the finest mesh level, get the electrostatic energy due to the interaction of the mobile charges with the potential and polarization of the dielectric medium:

$$G = \frac{1}{4I_s} \sum_i c_i q_i^2 \int \bar{\kappa}^2(x) e^{-q_i u(x)} dx + \frac{1}{2} \int \epsilon (\nabla u)^2 dx$$

for the NPBE and

$$G = \frac{1}{2} \int \bar{\kappa}^2(x) u^2(x) dx + \frac{1}{2} \int \epsilon (\nabla u)^2 dx$$

for the LPBE. Here i denotes the counterion species, I_s is the bulk ionic strength, $\bar{\kappa}^2(x)$ is the modified Debye-Huckel parameter, c_i is the concentration of species i , q_i is the charge of species i , ϵ is the dielectric function, and $u(x)$ is the dimensionless electrostatic potential. The energy is scaled to units of $k_b T$.

Author

Nathan Baker

Parameters

<i>thee</i>	Vfetc object
<i>color</i>	Partition restriction for energy evaluation, only used if non-negative

Returns

The "mobile charge" and "polarization" contributions to the electrostatic energy in units of $k_B T$.

Parameters

<i>thee</i>	The Vfetc object
<i>color</i>	Partition restriction for energy calculation; if non-negative, energy calculation is restricted to the specified partition (indexed by simplex and atom colors)

Definition at line 842 of file [vfetc.c](#).

7.3.5.5 Vfetc_dtor()

```
VEXTERNC void Vfetc_dtor (
    Vfetc ** thee )
```

Object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to memory location of Vfetk object
-------------	--

Definition at line 625 of file [vfetk.c](#).

7.3.5.6 Vfetk_dtor2()

```
VEXTERNC void Vfetk_dtor2 (
    Vfetk * thee )
```

FORTTRAN stub object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to Vfetk object to be destroyed
-------------	---

Definition at line 633 of file [vfetk.c](#).

7.3.5.7 Vfetk_dumpLocalVar()

```
VEXTERNC void Vfetk_dumpLocalVar ( )
```

Debugging routine to print out local variables used by PDE object.

Author

Nathan Baker

Bug This function is not thread-safe

Definition at line 2255 of file [vfetk.c](#).

7.3.5.8 Vfetk_energy()

```
VEXTERNC double Vfetk_energy (
    Vfetk * thee,
    int color,
    int nonlin )
```

Return the total electrostatic energy.

Using the solution at the finest mesh level, get the electrostatic energy using the free energy functional for the Poisson-Boltzmann equation without removing any self-interaction terms (i.e., removing the reference state of isolated charges present in an infinite dielectric continuum with the same relative permittivity as the interior of the protein) and return the result in units of $k_B T$. The argument *color* allows the user to control the partition on which this energy is calculated; if (*color* == -1) no restrictions are used. The solution is obtained from the finest level of the passed AM object, but atomic data from the Vfetk object is used to calculate the energy.

Author

Nathan Baker

ReturnsTotal electrostatic energy in units of $k_B T$.

< Total energy

<

<

Parameters

<i>thee</i>	The Vfetk object
<i>color</i>	Partition restriction for energy calculation; if non-negative, energy calculation is restricted to the specified partition (indexed by simplex and atom colors)
<i>nonlin</i>	If 1, the NPBE energy functional is used; otherwise, the LPBE energy functional is used. If -2, SMPBE is used.

Definition at line 693 of file [vfetk.c](#).**7.3.5.9 Vfetk_externalUpdateFunction()**

```

VEXTERNC void Vfetk_externalUpdateFunction (
    SS ** simps,
    int num )

```

External hook to simplex subdivision routines in Gem. Called each time a simplex is subdivided (we use it to update the charge-simplex map)

Author

Nathan Baker

Bug This function is not thread-safe.**Parameters**

<i>simps</i>	List of parent (<i>simps</i> [0]) and children (remainder) simplices
<i>num</i>	Number of simplices in list

Definition at line 2078 of file [vfetk.c](#).**7.3.5.10 Vfetk_fillArray()**

```

VEXTERNC int Vfetk_fillArray (
    Vfetk * thee,
    Bvec * vec,
    Vdata_Type type )

```

Fill an array with the specified data.

Author

Nathan Baker

Note

This function is thread-safe

Bug Several values of type are not implemented

Returns

1 if successful, 0 otherwise

Parameters

<i>thee</i>	The Vfetk object with the data
<i>vec</i>	The vector to hold the data
<i>type</i>	The type of data to write

Definition at line 2299 of file [vfetk.c](#).

7.3.5.11 Vfetk_genCube()

```
VEXTERNC Vrc_Codes Vfetk_genCube (
    Vfetk * thee,
    double center[3],
    double length[3],
    Vfetk_MeshLoad meshType )
```

Construct a rectangular mesh (in the current Vfetk object)

Author

Nathan Baker

Generates a new cube mesh within the provided Vfetk object based on the specified mesh type. Creates a new copy of the mesh based on the global variables at the top of the file and the mesh type, then recenters the mesh based on the center and length variables provided to the function.

Parameters

<i>thee</i>	Vfetk object
<i>center</i>	Center for mesh, which the new mesh will adjust to
<i>length</i>	Mesh lengths, which the new mesh will adjust to
<i>meshType</i>	Mesh boundary conditions

Definition at line 885 of file [vfetk.c](#).

7.3.5.12 Vfetk_getAM()

```
VEXTERNC AM * Vfetk_getAM (
    Vfetk * thee )
```

Get a pointer to the AM (algebra manager) object.

Author

Nathan Baker

Returns

Pointer to the AM (algebra manager) object

Parameters

<i>thee</i>	The Vfetk object
-------------	------------------

Definition at line 497 of file [vfetk.c](#).

7.3.5.13 Vfetk_getAtomColor()

```
VEXTERNC int Vfetk_getAtomColor (
    Vfetk * thee,
    int iatom )
```

Get the partition information for a particular atom.

Author

Nathan Baker

Note

Friend function of Vatom

Returns

Partition ID

Parameters

<i>thee</i>	The Vfetk object
<i>iatom</i>	Valist atom index

Definition at line 517 of file [vfetk.c](#).

7.3.5.14 Vfetk_getGem()

```
VEXTERNC Gem * Vfetk_getGem (
    Vfetk * thee )
```

Get a pointer to the Gem (grid manager) object.

Author

Nathan Baker

Returns

Pointer to the Gem (grid manager) object

Parameters

<i>thee</i>	Vfetk object
-------------	--------------

Definition at line 490 of file [vfetk.c](#).

7.3.5.15 Vfetk_getSolution()

```
VEXTERNC double * Vfetk_getSolution (
    Vfetk * thee,
    int * length )
```

Create an array containing the solution (electrostatic potential in units of $k_B T/e$) at the finest mesh level.

Author

Nathan Baker and Michael Holst

Note

The user is responsible for destroying the newly created array

Returns

Newly created array of length "length" (see above); the user is responsible for destruction

Parameters

<i>thee</i>	Vfetk object with solution
<i>length</i>	Ste to length of the newly created solution array

Definition at line 641 of file [vfetk.c](#).

7.3.5.16 Vfetk_getVcsm()

```
VEXTERNC Vcsm * Vfetk_getVcsm (
    Vfetk * thee )
```

Get a pointer to the Vcsm (charge-simplex map) object.

Author

Nathan Baker

Returns

Pointer to the Vcsm (charge-simplex map) object

Parameters

<i>thee</i>	The Vfetk object
-------------	------------------

Definition at line 510 of file [vfetk.c](#).

7.3.5.17 Vfetk_getVpbe()

```
VEXTERNC Vpbe * Vfetk_getVpbe (
    Vfetk * thee )
```

Get a pointer to the Vpbe (PBE manager) object.

Author

Nathan Baker

Returns

Pointer to the Vpbe (PBE manager) object

Parameters

<i>thee</i>	The Vfetk object
-------------	------------------

Definition at line 503 of file [vfetk.c](#).**7.3.5.18 Vfetk_loadGem()**

```

VEXTERNC Vrc_Codes Vfetk_loadGem (
    Vfetk * thee,
    Gem * gm )

```

Load a Gem geometry manager object into Vfetk.

Author

Nathan Baker

Parameters

<i>thee</i>	Destination
<i>gm</i>	Geometry manager source

7.3.5.19 Vfetk_loadMesh()

```

VEXTERNC Vrc_Codes Vfetk_loadMesh (
    Vfetk * thee,
    double center[3],
    double length[3],
    Vfetk_MeshLoad meshType,
    Vio * sock )

```

Loads a mesh into the Vfetk (and associated) object(s).

Author

Nathan Baker

If we have an external mesh, load that external mesh from the provided socket. If we specify a non-external mesh type, we generate a new mesh cube based on templates. We then create and store a new Vcsm object in our Vfetk structure, which will carry the mesh data.

Parameters

<i>thee</i>	Vfetk object to load into
<i>center</i>	Center for mesh (if constructed)
<i>length</i>	Mesh lengths (if constructed)
<i>meshType</i>	Type of mesh to load
<i>sock</i>	Socket for external mesh data (NULL otherwise)

Definition at line 980 of file [vfetc.c](#).

7.3.5.20 Vfetc_memChk()

```
VEXTERNC unsigned long int Vfetc_memChk (
    Vfetc * thee )
```

Return the memory used by this structure (and its contents) in bytes.

Author

Nathan Baker

Returns

The memory used by this structure and its contents in bytes

Parameters

<i>thee</i>	The Vfetc object
-------------	------------------

Definition at line 867 of file [vfetc.c](#).

7.3.5.21 Vfetc_PDE_bisectEdge()

```
VEXTERNC void Vfetc_PDE_bisectEdge (
    int dim,
    int dimII,
    int edgeType,
    int chart[],
    double vx[][VAPBS_DIM] )
```

Define the way manifold edges are bisected.

Author

Nathan Baker and Mike Holst

Note

This function is thread-safe.

Parameters

<i>dim</i>	Intrinsic dimension of manifold
<i>dimII</i>	Embedding dimension of manifold
<i>edgeType</i>	Type of edge being refined
<i>chart</i>	Chart for edge vertices, used here as accessibility bitfields
<i>vx</i>	Edge vertex coordinates

7.3.5.22 Vfetc_PDE_ctor()

```
VEXTERNC PDE * Vfetc_PDE_ctor (
    Vfetc * fetk )
```

Constructs the FEtk PDE object.

Author

Nathan Baker

Returns

Newly-allocated PDE object

Bug Not thread-safe**Parameters**

<i>fetk</i>	The Vfetk object
-------------	------------------

Definition at line 1176 of file [vfetk.c](#).**7.3.5.23 Vfetk_PDE_ctor2()**

```
VEXTERNC int Vfetk_PDE_ctor2 (
    PDE * thee,
    Vfetk * fetk )
```

Initializes the FETk PDE object.

Author

Nathan Baker (with code by Mike Holst)

Returns

1 if successful, 0 otherwise

Bug Not thread-safe**Parameters**

<i>thee</i>	The newly-allocated PDE object
<i>fetk</i>	The parent Vfetk object

Definition at line 1187 of file [vfetk.c](#).**7.3.5.24 Vfetk_PDE_delta()**

```
VEXTERNC void Vfetk_PDE_delta (
    PDE * thee,
    int type,
    int chart,
    double txq[],
    void * user,
    double F[] )
```

Evaluate a (discretized) delta function source term at the given point.

Author

Nathan Baker

Bug This function is not thread-safe

Parameters

<i>thee</i>	PDE object
<i>type</i>	Vertex type
<i>chart</i>	Chart for point coordinates
<i>txq</i>	Point coordinates
<i>user</i>	Vertex object pointer
<i>F</i>	Set to delta function value

Definition at line 1780 of file [vfetk.c](#).

7.3.5.25 Vfetk_PDE_DFu_wv()

```

VEXTERNC double Vfetk_PDE_DFu_wv (
    PDE * thee,
    int key,
    double W[],
    double dW[][VAPBS_DIM],
    double V[],
    double dV[][VAPBS_DIM] )

```

This is the linearization of the weak form of the PBE; e.g., for use in a Newton iteration. This is the functional linearization of the strong form integrated with a test function to give:

$$\int_{\Omega} [\epsilon \nabla w \cdot \nabla v + b'(u) w v - f v] dx$$

where $b'(u)$ denotes the functional derivation of the mobile ion term.

Author

Nathan Baker and Mike Holst

Returns

Integrand value

Bug This function is not thread-safe

Parameters

<i>thee</i>	The PDE object
<i>key</i>	Integrand to evaluate (0 = interior weak form, 1 = boundary weak form)
<i>W</i>	Trial function value at current point
<i>dW</i>	Trial function gradient at current point
<i>V</i>	Test function value at current point
<i>dV</i>	Test function gradient

7.3.5.26 Vfetk_PDE_dtor()

```

VEXTERNC void Vfetk_PDE_dtor (
    PDE ** thee )

```

Destroys FETk PDE object.

Author

Nathan Baker

Note

Thread-safe

Parameters

<i>thee</i>	Pointer to PDE object memory
-------------	------------------------------

Definition at line 1231 of file [vfetk.c](#).**7.3.5.27 Vfetk_PDE_dtor2()**

```
VEXTERNC void Vfetk_PDE_dtor2 (
    PDE * thee )
```

FORTRAN stub: destroys FEtk PDE object.

Author

Nathan Baker

Note

Thread-safe

Parameters

<i>thee</i>	PDE object memory
-------------	-------------------

Definition at line 1246 of file [vfetk.c](#).**7.3.5.28 Vfetk_PDE_Fu()**

```
VEXTERNC void Vfetk_PDE_Fu (
    PDE * thee,
    int key,
    double F[] )
```

Evaluate strong form of PBE. For interior points, this is:

$$-\nabla \cdot \epsilon \nabla u + b(u) - f$$

where $b(u)$ is the (possibly nonlinear) mobile ion term and f is the source charge distribution term (for PBE) or the induced surface charge distribution (for RPBE). For an interior-boundary (simplex face) point, this is:

$$[\epsilon(x) \nabla u(x) \cdot n(x)]_{x=0+} - [\epsilon(x) \nabla u(x) \cdot n(x)]_{x=0-}$$

where $n(x)$ is the normal to the simplex face and the term represents the jump in dielectric displacement across the face. There is no outer-boundary contribution for this problem.

Author

Nathan Baker

Bug This function is not thread-safe

This function is not implemented (sets error to zero)

Parameters

<i>thee</i>	The PDE object
<i>key</i>	Type of point (0 = interior, 1 = boundary, 2 = interior boundary)
<i>F</i>	Set to value of residual

Definition at line 1695 of file [vfetk.c](#).

7.3.5.29 Vfetk_PDE_Fu_v()

```

VEXTERNC double Vfetk_PDE_Fu_v (
    PDE * thee,
    int key,
    double V[],
    double dV[][VAPBS_DIM] )

```

This is the weak form of the PBE; i.e. the strong form integrated with a test function to give:

$$\int_{\Omega} [\epsilon \nabla u \cdot \nabla v + b(u)v - fv] dx$$

where $b(u)$ denotes the mobile ion term.

Author

Nathan Baker and Mike Holst

Returns

Integrand value

Bug This function is not thread-safe

Parameters

<i>thee</i>	The PDE object
<i>key</i>	Integrand to evaluate (0 = interior weak form, 1 = boundary weak form)
<i>V</i>	Test function at current point
<i>dV</i>	Test function derivative at current point

Definition at line 1703 of file [vfetk.c](#).

7.3.5.30 Vfetk_PDE_initAssemble()

```

VEXTERNC void Vfetk_PDE_initAssemble (
    PDE * thee,
    int ip[],
    double rp[] )

```

Do once-per-assembly initialization.

Author

Nathan Baker and Mike Holst

Note

Thread-safe

Parameters

<i>thee</i>	PDE object
<i>ip</i>	Integer parameter array (not used)
<i>rp</i>	Double parameter array (not used)

Definition at line 1508 of file [vfetk.c](#).

7.3.5.31 Vfetk_PDE_initElement()

```

VEXTERNC void Vfetk_PDE_initElement (
    PDE * thee,
    int elementType,
    int chart,
    double tvx[][VAPBS_DIM],
    void * data )

```

Do once-per-element initialization.

Author

Nathan Baker and Mike Holst

Bug This function is not thread-safe

Parameters

<i>thee</i>	PDE object
<i>elementType</i>	Material type (not used)
<i>chart</i>	Chart in which the vertex coordinates are provided, used here as a bitfield to store molecular accessibility
<i>tvx</i>	Vertex coordinates
<i>data</i>	Simplex pointer (hack)

7.3.5.32 Vfetk_PDE_initFace()

```

VEXTERNC void Vfetk_PDE_initFace (
    PDE * thee,
    int faceType,
    int chart,
    double tnvec[] )

```

Do once-per-face initialization.

Author

Nathan Baker and Mike Holst

Bug This function is not thread-safe

Parameters

<i>thee</i>	The PDE object
<i>faceType</i>	Simplex face type (interior or various boundary types)
<i>chart</i>	Chart in which the vertex coordinates are provided, used here as a bitfield for molecular accessibility
<i>tnvec</i>	Coordinates of outward normal vector for face

Definition at line 1559 of file [vfetk.c](#).

7.3.5.33 Vfetk_PDE_initPoint()

```

VEXTERNC void Vfetk_PDE_initPoint (
    PDE * thee,
    int pointType,
    int chart,
    double txq[],
    double tU[],
    double tdU[][VAPBS_DIM] )

```

Do once-per-point initialization.

Author

Nathan Baker

Bug This function is not thread-safe

This function uses pre-defined boudnary definitions for the molecular surface.

Parameters

<i>thee</i>	The PDE object
<i>pointType</i>	The type of point – interior or various faces
<i>chart</i>	The chart in which the point coordinates are provided, used here as bitfield for molecular accessibility
<i>txq</i>	Point coordinates
<i>tU</i>	Solution value at point
<i>tdU</i>	Solution derivative at point

7.3.5.34 Vfetk_PDE_Ju()

```

VEXTERNC double Vfetk_PDE_Ju (
    PDE * thee,
    int key )

```

Energy functional. This returns the energy (less delta function terms) in the form:

$$c^{-1}/2 \int (\epsilon(\nabla u)^2 + \kappa^2(\cosh u - 1)) dx$$

for a 1:1 electrolyte where c is the output from `Vpbe_getZmagic`.

Author

Nathan Baker

Returns

Energy value (in kT)

Bug This function is not thread-safe.

Parameters

<i>thee</i>	The PDE object
<i>key</i>	What to evaluate: interior (0) or boundary (1)?

Definition at line 2003 of file [vfetk.c](#).

7.3.5.35 Vfetk_PDE_mapBoundary()

```

VEXTERNC void Vfetk_PDE_mapBoundary (
    int dim,
    int dimII,
    int vertexType,
    int chart,
    double vx[VAPBS_DIM] )

```

Map a boundary point to some pre-defined shape.

Author

Nathan Baker and Mike Holst

Note

This function is thread-safe and is a no-op

Parameters

<i>dim</i>	Intrinsic dimension of manifold
<i>dimII</i>	Embedding dimension of manifold
<i>vertexType</i>	Type of vertex
<i>chart</i>	Chart for vertex coordinates
<i>vx</i>	Vertex coordinates

7.3.5.36 Vfetk_PDE_markSimplex()

```

VEXTERNC int Vfetk_PDE_markSimplex (
    int dim,
    int dimII,
    int simplexType,
    int faceType[VAPBS_NVS],
    int vertexType[VAPBS_NVS],
    int chart[],
    double vx[][VAPBS_DIM],
    void * simplex )

```

User-defined error estimator – in our case, a geometry-based refinement method; forcing simplex refinement at the dielectric boundary and (for non-regularized PBE) the charges.

Author

Nathan Baker

Returns

1 if mark simplex for refinement, 0 otherwise

Bug This function is not thread-safe**Parameters**

<i>dim</i>	Intrinsic manifold dimension
<i>dimII</i>	Embedding manifold dimension
<i>simplexType</i>	Type of simplex being refined
<i>faceType</i>	Types of faces in simplex
<i>vertexType</i>	Types of vertices in simplex
<i>chart</i>	Charts for vertex coordinates
<i>vx</i>	Vertex coordinates
<i>simplex</i>	Simplex pointer

7.3.5.37 Vfetc_PDE_oneChart()

```

VEXTERNC void Vfetc_PDE_oneChart (
    int dim,
    int dimII,
    int objType,
    int chart[],
    double vx[][VAPBS_DIM],
    int dimV )

```

Unify the chart for different coordinate systems – a no-op for us.

Author

Nathan Baker

Note

Thread-safe; a no-op

Parameters

<i>dim</i>	Intrinsic manifold dimension
<i>dimII</i>	Embedding manifold dimension
<i>objType</i>	???
<i>chart</i>	Charts of vertices' coordinates
<i>vx</i>	Vertices' coordinates
<i>dimV</i>	Number of vertices

7.3.5.38 Vfetk_PDE_simplexBasisForm()

```

VEXTERNC void Vfetk_PDE_simplexBasisForm (
    int key,
    int dim,
    int comp,
    int pdkey,
    double xq[],
    double basis[] )

```

Evaluate the bases for the trial or test space, for a particular component of the system, at all quadrature points on the master simplex element.

Author

Mike Holst

Parameters

<i>key</i>	Basis type to evaluate (0 = trial, 1 = test, 2 = trialB, 3 = testB)
<i>dim</i>	Spatial dimension
<i>comp</i>	Which component of elliptic system to produce basis for
<i>pdkey</i>	Basis partial differential equation evaluation key: <ul style="list-style-type: none"> • 0 = evaluate basis(x,y,z) • 1 = evaluate basis_x(x,y,z) • 2 = evaluate basis_y(x,y,z) • 3 = evaluate basis_z(x,y,z) • 4 = evaluate basis_xx(x,y,z) • 5 = evaluate basis_yy(x,y,z) • 6 = evaluate basis_zz(x,y,z) • 7 = etc...
<i>xq</i>	Set to quad pt coordinate
<i>basis</i>	Set to all basis functions evaluated at all quadrature pts

Definition at line [2203](#) of file [vfetk.c](#).

7.3.5.39 Vfetk_PDE_simplexBasisInit()

```

VEXTERNC int Vfetk_PDE_simplexBasisInit (
    int key,
    int dim,
    int comp,
    int * ndof,
    int dof[] )

```

Initialize the bases for the trial or the test space, for a particular component of the system, at all quadrature points on the master simplex element.

Author

Mike Holst

Note

```

* The basis ordering is important. For a fixed quadrature
* point iq, you must follow the following ordering in p[iq][],
* based on how you specify the degrees of freedom in dof[]:
*
* <v_0 vDF_0>,      <v_1 vDF_0>,      ..., <v_{nv} vDF_0>
* <v_0 vDF_1>,      <v_1 vDF_1>,      ..., <v_{nv} vDF_1>
*
*      ...
* <v_0 vDF_{nvDF}>, <v_0 vDF_{nvDF}>, ..., <v_{nv} vDF_{nvDF}>
*
* <e_0 eDF_0>,      <e_1 eDF_0>,      ..., <e_{ne} eDF_0>
* <e_0 eDF_1>,      <e_1 eDF_1>,      ..., <e_{ne} eDF_1>
*
*      ...
* <e_0 eDF_{neDF}>, <e_1 eDF_{neDF}>, ..., <e_{ne} eDF_{neDF}>
*
* <f_0 fDF_0>,      <f_1 fDF_0>,      ..., <f_{nf} fDF_0>
* <f_0 fDF_1>,      <f_1 fDF_1>,      ..., <f_{nf} fDF_1>
*
*      ...
* <f_0 fDF_{nfDF}>, <f_1 fDF_{nfDF}>, ..., <f_{nf} fDF_{nfDF}>
*
* <s_0 sDF_0>,      <s_1 sDF_0>,      ..., <s_{ns} sDF_0>
* <s_0 sDF_1>,      <s_1 sDF_1>,      ..., <s_{ns} sDF_1>
*
*      ...
* <s_0 sDF_{nsDF}>, <s_1 sDF_{nsDF}>, ..., <s_{ns} sDF_{nsDF}>
*
* For example, linear elements in R^3, with one degree of freedom at each
* vertex, would use the following ordering:
*
* <v_0 vDF_0>, <v_1 vDF_0>, <v_2 vDF_0>, <v_3 vDF_0>
*
* Quadratic elements in R^2, with one degree of freedom at each vertex and
* edge, would use the following ordering:
*
* <v_0 vDF_0>, <v_1 vDF_0>, <v_2 vDF_0>
* <e_0 eDF_0>, <e_1 eDF_0>, <e_2 eDF_0>
*
* You can use different trial and test spaces for each component of the
* elliptic system, thereby allowing for the use of Petrov-Galerkin methods.
* You MUST then tag the bilinear form symmetry entries as nonsymmetric in
* your PDE constructor to reflect that DF(u)(w,v) will be different from
* DF(u)(v,w), even if your form acts symmetrically when the same basis is
* used for w and v.
*
* You can also use different trial spaces for each component of the elliptic
* system, and different test spaces for each component of the elliptic
* system. This allows you to e.g. use a basis which is vertex-based for
* one component, and a basis which is edge-based for another. This is
* useful in fluid mechanics, eletromagnetics, or simply to play around with
* different elements.
*
* This function is called by MC to build new master elements whenever it
* reads in a new mesh. Therefore, this function does not have to be all
* that fast, and e.g. could involve symbolic computation.

```

Parameters

<i>key</i>	Basis type to evaluate (0 = trial, 1 = test, 2 = trialB, 3 = testB)
<i>dim</i>	Spatial dimension
<i>comp</i>	Which component of elliptic system to produce basis for?

Parameters

<i>ndof</i>	Set to the number of degrees of freedom
<i>dof</i>	Set to degree of freedom per v/e/f/s

Definition at line 2140 of file [vfetk.c](#).

7.3.5.40 Vfetk_PDE_u_D()

```

VEXTERNC void Vfetk_PDE_u_D (
    PDE * thee,
    int type,
    int chart,
    double txq[],
    double F[] )

```

Evaluate the Dirichlet boundary condition at the given point.

Author

Nathan Baker

Bug This function is hard-coded to call only multiple-sphere Debye-Hü functions.
This function is not thread-safe.

Parameters

<i>thee</i>	PDE object
<i>type</i>	Vertex boundary type
<i>chart</i>	Chart for point coordinates
<i>txq</i>	Point coordinates
<i>F</i>	Set to boundary values

Definition at line 1867 of file [vfetk.c](#).

7.3.5.41 Vfetk_PDE_u_T()

```

VEXTERNC void Vfetk_PDE_u_T (
    PDE * thee,
    int type,
    int chart,
    double txq[],
    double F[] )

```

Evaluate the "true solution" at the given point for comparison with the numerical solution.

Author

Nathan Baker

Note

This function only returns zero.

Bug This function is not thread-safe.

The signature here doesn't match what's in mc's src/pde/mc/pde.h, which g++ seems to dislike for GAMer integration. Trying a change of function signature to match to see if that makes g++ happy. Also see [vfetk.h](#) for similar signature change. - P. Ellis 11-8-2011

Parameters

<i>thee</i>	PDE object
<i>type</i>	Point type
<i>chart</i>	Chart for point coordinates
<i>txq</i>	Point coordinates
<i>F</i>	Set to value at point

Definition at line 1886 of file [vfetk.c](#).

7.3.5.42 Vfetk_qfEnergy()

```
VEXTERNC double Vfetk_qfEnergy (
    Vfetk * thee,
    int color )
```

Get the "fixed charge" contribution to the electrostatic energy.

Using the solution at the finest mesh level, get the electrostatic energy due to the interaction of the fixed charges with the potential: $G = \sum_i q_i u(r_i)$ and return the result in units of $k_B T$. Clearly, no self-interaction terms are removed. A factor a 1/2 has to be included to convert this to a real energy.

Author

Nathan Baker

Parameters

<i>thee</i>	Vfetk object
<i>color</i>	Partition restriction for energy evaluation, only used if non-negative

Returns

The fixed charge electrostatic energy in units of $k_B T$.

Parameters

<i>thee</i>	The Vfetk object
<i>color</i>	Partition restriction for energy evaluation, only used if non-negative

Definition at line 732 of file [vfetk.c](#).

7.3.5.43 Vfetk_readMesh()

```
VEXTERNC void Vfetk_readMesh (
    Vfetk * thee,
```



```
int skey,
Vio * sock )
```

Read in mesh and initialize associated internal structures.

Author

Nathan Baker

Note

See also

[Vfetk_genCube](#)

Parameters

<i>thee</i>	The Vfetk object
<i>skey</i>	The sock format key (0 = MCSF simplex format)
<i>sock</i>	Socket object ready for reading

7.3.5.44 Vfetk_setAtomColors()

```
VEEXTERNC void Vfetk_setAtomColors (
    Vfetk * thee )
```

Transfer color (partition ID) information from a partitioned mesh to the atoms.

Transfer color information from partitioned mesh to the atoms. In the case that a charge is shared between two partitions, the partition color of the first simplex is selected. Due to the arbitrary nature of this selection, THIS METHOD SHOULD ONLY BE USED IMMEDIATELY AFTER PARTITIONING!!!

Warning

This function should only be used immediately after mesh partitioning

Author

Nathan Baker

Note

This is a friend function of Vcsm

Parameters

<i>thee</i>	The Vfetk object
-------------	------------------

Definition at line [849](#) of file [vfetk.c](#).

7.3.5.45 Vfetk_setParameters()

```
VEEXTERNC void Vfetk_setParameters (
    Vfetk * thee,
```

```
PBEparm * pbeparm,
FEMparm * feparm )
```

Set the parameter objects.

Author

Nathan Baker

Parameters

<i>thee</i>	The Vfetk object
<i>pbeparm</i>	Parameters for solution of the PBE
<i>feparm</i>	FEM-specific solution parameters

Definition at line 615 of file [vfetk.c](#).

7.3.5.46 Vfetk_write()

```
VEXTERNC int Vfetk_write (
    Vfetk * thee,
    const char * iodev,
    const char * iofmt,
    const char * thost,
    const char * fname,
    Bvec * vec,
    Vdata_Format format )
```

Write out data.

Author

Nathan Baker

Parameters

<i>thee</i>	Vfetk object
<i>vec</i>	FEtk Bvec vector to use
<i>format</i>	Format for data
<i>iodev</i>	Output device type (FILE/BUFF/UNIX/INET)
<i>iofmt</i>	Output device format (ASCII/XDR)
<i>thost</i>	Output hostname (for sockets)
<i>fname</i>	Output FILE/BUFF/UNIX/INET name

Note

This function is thread-safe

Bug Some values of format are not implemented

Returns

1 if successful, 0 otherwise

Parameters

<i>thee</i>	The Vfetc object
<i>iodev</i>	Output device type (FILE = file, BUFF = buffer, UNIX = unix pipe, INET = network socket)
<i>iofmt</i>	Output device format (ASCII = ascii/plaintext, XDR = xdr)
<i>thost</i>	Output hostname for sockets
<i>fname</i>	Output filename for other
<i>vec</i>	Data vector
<i>format</i>	Data format

Definition at line 2464 of file [vfetc.c](#).

7.4 Vpee class

This class provides some functionality for error esimation in parallel.

Files

- file [vpee.c](#)
Class Vpee methods.
- file [vpee.h](#)
Contains declarations for class Vpee.

Data Structures

- struct [sVpee](#)
Contains public data members for Vpee class/module.

Typedefs

- typedef struct [sVpee](#) [Vpee](#)
Declaration of the Vpee class as the Vpee structure.

Functions

- VEXTERNC [Vpee](#) * [Vpee_ctor](#) (Gem *gm, int localPartID, int killFlag, double killParam)
Construct the Vpee object.
- VEXTERNC int [Vpee_ctor2](#) ([Vpee](#) *thee, Gem *gm, int localPartID, int killFlag, double killParam)
FORTTRAN stub to construct the Vpee object.
- VEXTERNC void [Vpee_dtor](#) ([Vpee](#) **thee)
Object destructor.
- VEXTERNC void [Vpee_dtor2](#) ([Vpee](#) *thee)
FORTTRAN stub object destructor.
- VEXTERNC int [Vpee_markRefine](#) ([Vpee](#) *thee, AM *am, int level, int akey, int rcol, double etol, int bkey)
Mark simplices for refinement based on attenuated error estimates.
- VEXTERNC int [Vpee_numSS](#) ([Vpee](#) *thee)
Returns the number of simplices in the local partition.

7.4.1 Detailed Description

This class provides some functionality for error esimation in parallel.

This class provides some functionality for error esimation in parallel. The purpose is to modulate the error returned by some external error estimator according to the partitioning of the mesh. For example, the Bank/Holst parallel refinement routine essentially reduces the error outside the local" partition to zero. However, this leads to the need for a few final overlapping Schwarz solves to smooth out the errors near partition boundaries. Supposedly, if the region in which we allow error-based refinement includes the"local" partition and an external buffer zone approximately equal in size to the local region, then the solution will asymptotically approach the solution obtained via more typical methods. This is essentially a more flexible parallel implementation of MC's AM_markRefine.

7.4.2 Typedef Documentation

7.4.2.1 Vpee

```
typedef struct sVpee Vpee
```

Declaration of the Vpee class as the Vpee structure.

Definition at line 112 of file [vpee.h](#).

7.4.3 Function Documentation

7.4.3.1 Vpee_ctor()

```
VEXTERNC Vpee * Vpee_ctor (
    Gem * gm,
    int localPartID,
    int killFlag,
    double killParam )
```

Construct the Vpee object.

Author

Nathan Baker

Returns

Newly constructed Vpee object

Parameters

<i>gm</i>	FEtk geometry manager object
<i>localPartID</i>	ID of the local partition (focus of refinement)
<i>killFlag</i>	A flag to indicate how error estimates are to be attenuated outside the local partition: <ul style="list-style-type: none"> • 0: no attenuation • 1: all error outside the local partition set to zero • 2: all error is set to zero outside a sphere of radius (killParam*partRadius), where partRadius is the radius of the sphere circumscribing the local partition • 3: all error is set to zero except for the local partition and its immediate neighbors
<i>killParam</i>	

See also

killFlag for usage

Definition at line 93 of file [vpee.c](#).

7.4.3.2 Vpee_ctor2()

```
VEXTERNC int Vpee_ctor2 (
    Vpee * thee,
    Gem * gm,
    int localPartID,
    int killFlag,
    double killParam )
```

FORTTRAN stub to construct the Vpee object.

Author

Nathan Baker

Returns

1 if successful, 0 otherwise

Parameters

<i>thee</i>	The Vpee object
<i>gm</i>	FETk geometry manager object
<i>localPartID</i>	ID of the local partition (focus of refinement)
<i>killFlag</i>	A flag to indicate how error estimates are to be attenuated outside the local partition: <ul style="list-style-type: none"> • 0: no attenuation • 1: all error outside the local partition set to zero • 2: all error is set to zero outside a sphere of radius (killParam*partRadius), where partRadius is the radius of the sphere circumscribing the local partition • 3: all error is set to zero except for the local partition and its immediate neighbors
<i>killParam</i>	

See also

killFlag for usage

Definition at line 114 of file [vpee.c](#).

7.4.3.3 Vpee_dtor()

```
VEXTERNC void Vpee_dtor (
    Vpee ** thee )
```

Object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to memory location of the Vpee object
-------------	---

Definition at line 225 of file [vpee.c](#).

7.4.3.4 Vpee_dtor2()

```

VEXTERNC void Vpee_dtor2 (
    Vpee * thee )

```

FORTTRAN stub object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to object to be destroyed
-------------	-----------------------------------

Definition at line 240 of file [vpee.c](#).

7.4.3.5 Vpee_markRefine()

```

VEXTERNC int Vpee_markRefine (
    Vpee * thee,
    AM * am,
    int level,
    int akey,
    int rcol,
    double etol,
    int bkey )

```

Mark simplices for refinement based on attenuated error estimates.

A wrapper/reimplementation of AM_markRefine that allows for more flexible attenuation of error-based markings outside the local partition. The error in each simplex is modified by the method (see killFlag) specified in the Vpee constructor. This allows the user to confine refinement to an arbitrary area around the local partition.

Author

Nathan Baker and Mike Holst

Note

This routine borrows very heavily from FEtk routines by Mike Holst.

Returns

The number of simplices marked for refinement.

Bug This function is no longer up-to-date with FEtk and may not function properly

Parameters

<i>thee</i>	The Vpee object
<i>am</i>	The FEtk algebra manager currently used to solve the PB

Parameters

<i>level</i>	The current level of the multigrid hierarchy
<i>akey</i>	The marking method: <ul style="list-style-type: none"> • -1: Reset markings --> killFlag has no effect. • 0: Uniform. • 1: User defined (geometry-based). • >1: A numerical estimate for the error has already been set in am and should be attenuated according to killFlag and used, in conjunction with etol, to mark simplices for refinement.
<i>rcol</i>	The ID of the main partition on which to mark (or -1 if all partitions should be marked). NOte that we shouldhave (rcol == thee->localPartID) for (thee->killFlag == 2 or 3)
<i>etol</i>	The error tolerance criterion for marking
<i>bkey</i>	How the error tolerance is interpreted: <ul style="list-style-type: none"> • 0: Simplex marked if error > etol. • 1: Simplex marked if error > sqrt(etol^2/L) where L\$ is the number of simplices

Definition at line 250 of file [vpee.c](#).

7.4.3.6 Vpee_numSS()

```

VEXTERNC int Vpee_numSS (
    Vpee * thee )

```

Returns the number of simplices in the local partition.

Author

Nathan Baker

Returns

Number of simplices in the local partition

Parameters

<i>thee</i>	The Vpee object
-------------	-----------------

Definition at line 479 of file [vpee.c](#).

7.5 APOLparm class

Parameter structure for APOL-specific variables from input files.

Files

- file [apolparm.c](#)
Class APOLparm methods.
- file [femparm.h](#)

Contains declarations for class APOLparm.

Data Structures

- struct [sAPOLparm](#)

Parameter structure for APOL-specific variables from input files.

Typedefs

- typedef enum [eAPOLparm_calcEnergy](#) [APOLparm_calcEnergy](#)
Define eAPOLparm_calcEnergy enumeration as APOLparm_calcEnergy.
- typedef enum [eAPOLparm_calcForce](#) [APOLparm_calcForce](#)
Define eAPOLparm_calcForce enumeration as APOLparm_calcForce.
- typedef enum [eAPOLparm_doCalc](#) [APOLparm_doCalc](#)
Define eAPOLparm_calcForce enumeration as APOLparm_calcForce.

Enumerations

- enum [eAPOLparm_calcEnergy](#) { [ACE_NO](#) =0 , [ACE_TOTAL](#) =1 , [ACE_COMPS](#) =2 }
Define energy calculation enumeration.
- enum [eAPOLparm_calcForce](#) { [ACF_NO](#) =0 , [ACF_TOTAL](#) =1 , [ACF_COMPS](#) =2 }
Define force calculation enumeration.
- enum [eAPOLparm_doCalc](#) { [ACD_NO](#) =0 , [ACD_YES](#) =1 , [ACD_ERROR](#) =2 }
Define force calculation enumeration.

Functions

- VEXTERNC [APOLparm](#) * [APOLparm_ctor](#) ()
Construct APOLparm.
- VEXTERNC Vrc_Codes [APOLparm_ctor2](#) ([APOLparm](#) *thee)
FORTTRAN stub to construct APOLparm.
- VEXTERNC void [APOLparm_dtor](#) ([APOLparm](#) **thee)
Object destructor.
- VEXTERNC void [APOLparm_dtor2](#) ([APOLparm](#) *thee)
FORTTRAN stub for object destructor.
- VEXTERNC Vrc_Codes [APOLparm_check](#) ([APOLparm](#) *thee)
Consistency check for parameter values stored in object.
- VEXTERNC void [APOLparm_copy](#) ([APOLparm](#) *thee, [APOLparm](#) *source)
Copy target object into thee.

7.5.1 Detailed Description

Parameter structure for APOL-specific variables from input files.

7.5.2 Typedef Documentation

7.5.2.1 APOLparm_calcEnergy

typedef enum [eAPOLparm_calcEnergy](#) [APOLparm_calcEnergy](#)
Define eAPOLparm_calcEnergy enumeration as APOLparm_calcEnergy.
Definition at line 89 of file [apolparm.h](#).

7.5.2.2 APOLparm_calcForce

typedef enum eAPOLparm_calcForce APOLparm_calcForce
Define eAPOLparm_calcForce enumeration as APOLparm_calcForce.
Definition at line 105 of file [apolparm.h](#).

7.5.2.3 APOLparm_doCalc

typedef enum eAPOLparm_doCalc APOLparm_doCalc
Define eAPOLparm_calcForce enumeration as APOLparm_calcForce.
Definition at line 121 of file [apolparm.h](#).

7.5.3 Enumeration Type Documentation

7.5.3.1 eAPOLparm_calcEnergy

enum eAPOLparm_calcEnergy
Define energy calculation enumeration.

Enumerator

ACE_NO	Do not perform energy calculation
ACE_TOTAL	Calculate total energy only
ACE_COMPS	Calculate per-atom energy components

Definition at line 79 of file [apolparm.h](#).

7.5.3.2 eAPOLparm_calcForce

enum eAPOLparm_calcForce
Define force calculation enumeration.

Enumerator

ACF_NO	Do not perform force calculation
ACF_TOTAL	Calculate total force only
ACF_COMPS	Calculate per-atom force components

Definition at line 95 of file [apolparm.h](#).

7.5.3.3 eAPOLparm_doCalc

enum eAPOLparm_doCalc
Define force calculation enumeration.

Enumerator

ACD_NO	Do not perform calculation
ACD_YES	Perform calculations
ACD_ERROR	Error setting up calculation

Definition at line 111 of file [apolparm.h](#).

7.5.4 Function Documentation

7.5.4.1 APOLparm_check()

```
VEXTERNC Vrc_Codes APOLparm_check (
    APOLparm * thee )
```

Consistency check for parameter values stored in object.

Author

David Gohara, Yong Huang

Parameters

<i>thee</i>	APOLparm object
-------------	-----------------

Returns

Success enumeration

Definition at line 179 of file [apolparm.c](#).

7.5.4.2 APOLparm_copy()

```
VEXTERNC void APOLparm_copy (
    APOLparm * thee,
    APOLparm * source )
```

Copy target object into thee.

Author

Nathan Baker

Parameters

<i>thee</i>	Destination object
<i>source</i>	Source object

Definition at line 108 of file [apolparm.c](#).

7.5.4.3 APOLparm_ctor()

```
VEXTERNC APOLparm * APOLparm_ctor ( )
```

Construct APOLparm.

Author

David Gohara

Returns

Newly allocated and initialized Vpmgp object

Definition at line 65 of file [apolparm.c](#).

7.5.4.4 APOLparm_ctor2()

```
VEXTERNC Vrc_Codes APOLparm_ctor2 (  
    APOLparm * thee )
```

FORTTRAN stub to construct APOLparm.

Author

David Gohara, Yong Huang

Parameters

<i>thee</i>	Pointer to allocated APOLparm object
-------------	--------------------------------------

Returns

Success enumeration

Definition at line 76 of file [apolparm.c](#).

7.5.4.5 APOLparm_dtor()

```
VEXTERNC void APOLparm_dtor (  
    APOLparm ** thee )
```

Object destructor.

Author

David Gohara

Parameters

<i>thee</i>	Pointer to memory location of APOLparm object
-------------	---

Definition at line 167 of file [apolparm.c](#).

7.5.4.6 APOLparm_dtor2()

```
VEXTERNC void APOLparm_dtor2 (  
    APOLparm * thee )
```

FORTTRAN stub for object destructor.

Author

David Gohara

Parameters

<i>thee</i>	Pointer to APOLparm object
-------------	----------------------------

Definition at line 177 of file [apolparm.c](#).

7.6 BEMparm class

Parameter which holds useful parameters for generic multigrid calculations.

Files

- file [bemparm.c](#)
Class BEMparm methods.

Data Structures

- struct [sBEMparm](#)
Parameter structure for BEM-specific variables from input files.

Typedefs

- typedef enum [eBEMparm_CalcType](#) [BEMparm_CalcType](#)
Declare BEMparm_CalcType type.
- typedef struct [sBEMparm](#) [BEMparm](#)
Parameter structure for BEM-specific variables from input files.

Enumerations

- enum [eBEMparm_CalcType](#) { [BCT_MANUAL](#) =0 , [BCT_NONE](#) =1 }
Calculation type.

Functions

- VEXTERNC [BEMparm](#) * [BEMparm_ctor](#) ([BEMparm_CalcType](#) type)
Construct BEMparm object.
- VEXTERNC Vrc_Codes [BEMparm_ctor2](#) ([BEMparm](#) *thee, [BEMparm_CalcType](#) type)
FORTTRAN stub to construct BEMparm object.
- VEXTERNC void [BEMparm_dtor](#) ([BEMparm](#) **thee)
Object destructor.
- VEXTERNC void [BEMparm_dtor2](#) ([BEMparm](#) *thee)
FORTTRAN stub for object destructor.
- VEXTERNC Vrc_Codes [BEMparm_check](#) ([BEMparm](#) *thee)
Consistency check for parameter values stored in object.
- VEXTERNC Vrc_Codes [BEMparm_parseToken](#) ([BEMparm](#) *thee, char tok[VMAX_BUFSIZE], Vio *sock)
Parse an MG keyword from an input file.

7.6.1 Detailed Description

Parameter which holds useful parameters for generic multigrid calculations.

7.6.2 Typedef Documentation

7.6.2.1 BEMparm

```
typedef struct sBEMparm BEMparm
```

Parameter structure for BEM-specific variables from input files.

Author

Nathan Baker and Todd Dolinsky and Weihua Geng

Note

If you add/delete/change something in this class, the member functions – especially `BEMparm_copy` – must be modified accordingly

7.6.2.2 BEMparm_CalcType

```
typedef enum eBEMparm_CalcType BEMparm_CalcType
```

Declare `BEMparm_CalcType` type.

Definition at line 86 of file [bemparm.h](#).

7.6.3 Enumeration Type Documentation**7.6.3.1 eBEMparm_CalcType**

```
enum eBEMparm_CalcType
```

Calculation type.

Enumerator

BCT_MANUAL	bem-manual
BCT_NONE	not defined

Definition at line 77 of file [bemparm.h](#).

7.6.4 Function Documentation**7.6.4.1 BEMparm_check()**

```
VEXTERNC Vrc_Codes BEMparm_check (
    BEMparm * thee )
```

Consistency check for parameter values stored in object.

Author

Nathan Baker

Parameters

<i>thee</i>	BEMparm object
-------------	----------------

Returns

Success enumeration

Definition at line 124 of file [bemparm.c](#).

7.6.4.2 BEMparm_ctor()

```
VEXTERNC BEMparm * BEMparm_ctor (
    BEMparm_CalcType type )
```

Construct BEMparm object.

Author

Nathan Baker

Parameters

<i>type</i>	Type of BEM calculation
-------------	-------------------------

Returns

Newly allocated and initialized BEMparm object

Definition at line 66 of file [bemparm.c](#).

7.6.4.3 BEMparm_ctor2()

```

VEXTERNC Vrc_Codes BEMparm_ctor2 (
    BEMparm * thee,
    BEMparm_CalcType type )

```

FORTTRAN stub to construct BEMparm object.

Author

Nathan Baker and Todd Dolinsky

Parameters

<i>thee</i>	Space for BEMparm object
<i>type</i>	Type of MG calculation

Returns

Success enumeration

Definition at line 77 of file [bemparm.c](#).

7.6.4.4 BEMparm_dtor()

```

VEXTERNC void BEMparm_dtor (
    BEMparm ** thee )

```

Object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to memory location of BEMparm object
-------------	--

Definition at line 114 of file [bemparm.c](#).

7.6.4.5 BEMparm_dtor2()

```

VEXTERNC void BEMparm_dtor2 (
    BEMparm * thee )

```

FORTTRAN stub for object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to BEMparm object
-------------	---------------------------

Definition at line 122 of file [bemparm.c](#).

7.6.4.6 BEMparm_parseToken()

```

VEXTERNC Vrc_Codes BEMparm_parseToken (
    BEMparm * thee,
    char tok[VMAX_BUFSIZE],
    Vio * sock )

```

Parse an MG keyword from an input file.

Author

Nathan Baker and Todd Dolinsky

Parameters

<i>thee</i>	BEMparm object
<i>tok</i>	Token to parse
<i>sock</i>	Stream for more tokens

Returns

Success enumeration (1 if matched and assigned; -1 if matched, but there's some sort of error (i.e., too few args); 0 if not matched)

Definition at line 332 of file [bemparm.c](#).

7.7 FEMparm class

Parameter structure for FEM-specific variables from input files.

Files

- file [femparm.c](#)
Class FEMparm methods.
- file [femparm.h](#)
Contains declarations for class APOLparm.

Data Structures

- struct [sFEMparm](#)

Parameter structure for FEM-specific variables from input files.

Typedefs

- typedef enum [eFEMparm_EtolType](#) [FEMparm_EtolType](#)
Declare FEMparm_EtolType type.
- typedef enum [eFEMparm_EstType](#) [FEMparm_EstType](#)
Declare FEMparm_EstType type.
- typedef enum [eFEMparm_CalcType](#) [FEMparm_CalcType](#)
Declare FEMparm_CalcType type.

Enumerations

- enum [eFEMparm_EtolType](#) { [FET_SIMP](#) =0 , [FET_GLOB](#) =1 , [FET_FRAC](#) =2 }
Adaptive refinement error estimate tolerance key.
- enum [eFEMparm_EstType](#) {
[FRT_UNIF](#) =0 , [FRT_GEOM](#) =1 , [FRT_RESI](#) =2 , [FRT_DUAL](#) =3 ,
[FRT_LOCA](#) =4 }
Adaptive refinement error estimator method.
- enum [eFEMparm_CalcType](#) { [FCT_MANUAL](#) , [FCT_NONE](#) }
Calculation type.

Functions

- VEXTERNC [FEMparm](#) * [FEMparm_ctor](#) ([FEMparm_CalcType](#) type)
Construct FEMparm.
- VEXTERNC int [FEMparm_ctor2](#) ([FEMparm](#) *thee, [FEMparm_CalcType](#) type)
FORTTRAN stub to construct FEMparm.
- VEXTERNC void [FEMparm_dtor](#) ([FEMparm](#) **thee)
Object destructor.
- VEXTERNC void [FEMparm_dtor2](#) ([FEMparm](#) *thee)
FORTTRAN stub for object destructor.
- VEXTERNC int [FEMparm_check](#) ([FEMparm](#) *thee)
Consistency check for parameter values stored in object.
- VEXTERNC void [FEMparm_copy](#) ([FEMparm](#) *thee, [FEMparm](#) *source)
Copy target object into thee.

7.7.1 Detailed Description

Parameter structure for FEM-specific variables from input files.

7.7.2 Typedef Documentation

7.7.2.1 FEMparm_CalcType

```
typedef enum eFEMparm\_CalcType FEMparm\_CalcType
```

Declare [FEMparm_CalcType](#) type.

Definition at line 126 of file [femparm.h](#).

7.7.2.2 FEMparm_EstType

`typedef enum eFEMparm_EstType FEMparm_EstType`
 Declare FEMparm_EstType type.
 Definition at line 111 of file [femparm.h](#).

7.7.2.3 FEMparm_EtolType

`typedef enum eFEMparm_EtolType FEMparm_EtolType`
 Declare FEparm_EtolType type.

Author

Nathan Baker

Definition at line 90 of file [femparm.h](#).

7.7.3 Enumeration Type Documentation

7.7.3.1 eFEMparm_CalcType

`enum eFEMparm_CalcType`
 Calculation type.

Enumerator

FCT_MANUAL	fe-manual
FCT_NONE	unspecified

Definition at line 117 of file [femparm.h](#).

7.7.3.2 eFEMparm_EstType

`enum eFEMparm_EstType`
 Adaptive refinement error estimator method.

Note

Do not change these values; they correspond to settings in FEtk

Author

Nathan Baker

Enumerator

FRT_UNIF	Uniform refinement
FRT_GEOM	Geometry-based (i.e. surfaces and charges) refinement
FRT_RESI	Nonlinear residual estimate-based refinement
FRT_DUAL	Dual-solution weight nonlinear residual estimate-based refinement
FRT_LOCA	Local problem error estimate-based refinement

Definition at line 98 of file [femparm.h](#).

7.7.3.3 eFEMparm_EtolType

enum [eFEMparm_EtolType](#)

Adaptive refinement error estimate tolerance key.

Author

Nathan Baker

Enumerator

FET_SIMP	per-simplex error tolerance
FET_GLOB	global error tolerance
FET_FRAC	fraction of simplices we want to have refined

Definition at line [79](#) of file [femparm.h](#).

7.7.4 Function Documentation

7.7.4.1 FEMparm_check()

```
VEXTERNC int FEMparm_check (
    FEMparm * thee )
```

Consistency check for parameter values stored in object.

Author

Nathan Baker

Parameters

<i>thee</i>	FEMparm object
-------------	----------------

Returns

1 if OK, 0 otherwise

Definition at line [143](#) of file [femparm.c](#).

7.7.4.2 FEMparm_copy()

```
VEXTERNC void FEMparm_copy (
    FEMparm * thee,
    FEMparm * source )
```

Copy target object into thee.

Author

Nathan Baker

Parameters

<i>thee</i>	Destination object
<i>source</i>	Source object

Definition at line 100 of file [femparm.c](#).

7.7.4.3 FEMparm_ctor()

```
VEXTERNC FEMparm * FEMparm_ctor (
    FEMparm_CalcType type )
```

Construct FEMparm.

Author

Nathan Baker

Parameters

<i>type</i>	FEM calculation type
-------------	----------------------

Returns

Newly allocated and initialized Vpmgp object

Definition at line 65 of file [femparm.c](#).

7.7.4.4 FEMparm_ctor2()

```
VEXTERNC int FEMparm_ctor2 (
    FEMparm * thee,
    FEMparm_CalcType type )
```

FORTTRAN stub to construct FEMparm.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to allocated FEMparm object
<i>type</i>	FEM calculation type

Returns

1 if successful, 0 otherwise

Definition at line 76 of file [femparm.c](#).

7.7.4.5 FEMparm_dtor()

```
VEXTERNC void FEMparm_dtor (
    FEMparm ** thee )
```

Object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to memory location of FEMparm object
-------------	--

Definition at line 133 of file [femparm.c](#).

7.7.4.6 FEMparm_dtor2()

```
VEXTERNC void FEMparm_dtor2 (
    FEMparm * thee )
```

FORTTRAN stub for object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to FEMparm object
-------------	---------------------------

Definition at line 141 of file [femparm.c](#).

7.8 GEOFLOWparm class

Parameter which holds useful parameters for GEOFLOWeric multigrid calculations.

Files

- file [geoflowparm.c](#)
Class GEOFLOWparm methods.
- file [geoflowparm.h](#)
Contains declarations for class GEOFLOWparm.

Data Structures

- struct [sGEOFLOWparm](#)
Parameter structure for GEOFLOW-specific variables from input files.

Typedefs

- typedef enum [eGEOFLOWparm_CalcType](#) [GEOFLOWparm_CalcType](#)
Declare GEOFLOWparm_CalcType type.
- typedef struct [sGEOFLOWparm](#) [GEOFLOWparm](#)
Parameter structure for GEOFLOW-specific variables from input files.

Enumerations

- enum [eGEOFLOWparm_CalcType](#) { [GFCT_AUTO](#) =1 }
Calculation type.

Functions

- VEXTERNC [GEOFLOWparm * GEOFLOWparm_ctor](#) ([GEOFLOWparm_CalcType](#) type)
Construct GEOFLOWparm object.
- VEXTERNC Vrc_Codes [GEOFLOWparm_ctor2](#) ([GEOFLOWparm *thee](#), [GEOFLOWparm_CalcType](#) type)
FORTRAN stub to construct GEOFLOWparm object ?????????!!!!!!
- VEXTERNC void [GEOFLOWparm_dtor](#) ([GEOFLOWparm **thee](#))
Object destructor.
- VEXTERNC void [GEOFLOWparm_dtor2](#) ([GEOFLOWparm *thee](#))
FORTRAN stub for object destructor ?????????!!!!!!
- VEXTERNC Vrc_Codes [GEOFLOWparm_check](#) ([GEOFLOWparm *thee](#))
Consistency check for parameter values stored in object.
- VEXTERNC Vrc_Codes [GEOFLOWparm_parseToken](#) ([GEOFLOWparm *thee](#), char tok[VMAX_BUFSIZE], Vio *sock)
Parse an MG keyword from an input file.
- VEXTERNC void [GEOFLOWparm_copy](#) ([GEOFLOWparm *thee](#), [GEOFLOWparm *parm](#))
copy GEOFLOWparm object into thee.

7.8.1 Detailed Description

Parameter which holds useful parameters for GEOFLOWeric multigrid calculations.

7.8.2 Typedef Documentation

7.8.2.1 GEOFLOWparm

```
typedef struct sGEOFLOWparm GEOFLOWparm
```

Parameter structure for GEOFLOW-specific variables from input files.

Author

Andrew Stevens, Kyle Monson

Note

If you add/delete/change something in this class, the member functions – especially [GEOFLOWparm_copy](#) – must be modified accordingly

7.8.2.2 GEOFLOWparm_CalcType

```
typedef enum eGEOFLOWparm_CalcType GEOFLOWparm_CalcType
```

Declare [GEOFLOWparm_CalcType](#) type.

Definition at line 88 of file [geoflowparm.h](#).

7.8.3 Enumeration Type Documentation

7.8.3.1 eGEOFLOWparm_CalcType

```
enum eGEOFLOWparm_CalcType
```

Calculation type.

Enumerator

GFCT_AUTO	GEOFLOW-auto
-----------	--------------

Definition at line 77 of file [geoflowparm.h](#).

7.8.4 Function Documentation

7.8.4.1 GEOFLOWparm_check()

```
VEXTERNC Vrc_Codes GEOFLOWparm_check (
    GEOFLOWparm * thee )
```

Consistency check for parameter values stored in object.

Author

Andrew Stevens, Kyle Monson

Parameters

<i>thee</i>	GEOFLOWparm object
-------------	--------------------

Returns

Success enumeration

Definition at line 101 of file [geoflowparm.c](#).

7.8.4.2 GEOFLOWparm_copy()

```
VEXTERNC void GEOFLOWparm_copy (
    GEOFLOWparm * thee,
    GEOFLOWparm * parm )
```

copy GEOFLOWparm object into thee.

Author

Parameters

<i>thee</i>	GEOFLOWparm object to be copied into
<i>parm</i>	GEOFLOWparm object.

Definition at line 127 of file [geoflowparm.c](#).

7.8.4.3 GEOFLOWparm_ctor()

```
VEXTERNC GEOFLOWparm * GEOFLOWparm_ctor (
    GEOFLOWparm_CalcType type )
```

Construct GEOFLOWparm object.

Author

Andrew Stevens, Kyle Monson

Parameters

<i>type</i>	Type of GEOFLOW calculation
-------------	-----------------------------

Returns

Newly allocated and initialized GEOFLOWparm object

Definition at line 66 of file [geoflowparm.c](#).

7.8.4.4 GEOFLOWparm_ctor2()

```

VEXTERNC Vrc_Codes GEOFLOWparm_ctor2 (
    GEOFLOWparm * thee,
    GEOFLOWparm_CalcType type )

```

FORTTRAN stub to construct GEOFLOWparm object ?????????!!!!!!!

Author

Andrew Stevens, Kyle Monson

Parameters

<i>thee</i>	Space for GEOFLOWparm object
<i>type</i>	Type of MG calculation

Returns

Success enumeration

Definition at line 77 of file [geoflowparm.c](#).

7.8.4.5 GEOFLOWparm_dtor()

```

VEXTERNC void GEOFLOWparm_dtor (
    GEOFLOWparm ** thee )

```

Object destructor.

Author

Andrew Stevens, Kyle Monson

Parameters

<i>thee</i>	Pointer to memory location of GEOFLOWparm object
-------------	--

Definition at line 91 of file [geoflowparm.c](#).

7.8.4.6 GEOFLOWparm_dtor2()

```

VEXTERNC void GEOFLOWparm_dtor2 (
    GEOFLOWparm * thee )

```

FORTTRAN stub for object destructor ?????????!!!!!!!

Author

Andrew Stevens, Kyle Monson

Parameters

<i>thee</i>	Pointer to GEOFLOWparm object
-------------	-------------------------------

Definition at line 99 of file [geoflowparm.c](#).

7.8.4.7 GEOFLOWparm_parseToken()

```
VEXTERNC Vrc_Codes GEOFLOWparm_parseToken (
    GEOFLOWparm * thee,
    char tok[VMAX_BUFSIZE],
    Vio * sock )
```

Parse an MG keyword from an input file.

Author

Andrew Stevens, Kyle Monson

Parameters

<i>thee</i>	GEOFLOWparm object
<i>tok</i>	Token to parse
<i>sock</i>	Stream for more tokens

Returns

Success enumeration (1 if matched and assigned; -1 if matched, but there's some sort of error (i.e., too few args); 0 if not matched)

Definition at line 212 of file [geoflowparm.c](#).

7.9 MGparm class

Parameter which holds useful parameters for generic multigrid calculations.

Files

- file [mgparm.c](#)
Class MGparm methods.
- file [mgparm.h](#)
Contains declarations for class MGparm.

Data Structures

- struct [sMGparm](#)
Parameter structure for MG-specific variables from input files.

Typedefs

- typedef enum [eMGparm_CalcType](#) MGparm_CalcType
Declare MGparm_CalcType type.
- typedef enum [eMGparm_CentMeth](#) MGparm_CentMeth
Declare MGparm_CentMeth type.

Enumerations

- enum `eMGparm_CalcType` {
`MCT_MANUAL` =0 , `MCT_AUTO` =1 , `MCT_PARALLEL` =2 , `MCT_DUMMY` =3 ,
`MCT_NONE` =4 }
- *Calculation type.*
- enum `eMGparm_CentMeth` { `MCM_POINT` =0 , `MCM_MOLECULE` =1 , `MCM_FOCUS` =2 }
- *Centering method.*

Functions

- VEXTERNC `Vrc_Codes` `APOLparm_parseToken` (`APOLparm` *thee, char tok[VMAX_BUFSIZE], `Vio` *sock)
Parse an MG keyword from an input file.
- VEXTERNC `Vrc_Codes` `FEMparm_parseToken` (`FEMparm` *thee, char tok[VMAX_BUFSIZE], `Vio` *sock)
Parse an MG keyword from an input file.
- VEXTERNC int `MGparm_getNx` (`MGparm` *thee)
Get number of grid points in x direction.
- VEXTERNC int `MGparm_getNy` (`MGparm` *thee)
Get number of grid points in y direction.
- VEXTERNC int `MGparm_getNz` (`MGparm` *thee)
Get number of grid points in z direction.
- VEXTERNC double `MGparm_getHx` (`MGparm` *thee)
Get grid spacing in x direction (Å)
- VEXTERNC double `MGparm_getHy` (`MGparm` *thee)
Get grid spacing in y direction (Å)
- VEXTERNC double `MGparm_getHz` (`MGparm` *thee)
Get grid spacing in z direction (Å)
- VEXTERNC void `MGparm_setCenterX` (`MGparm` *thee, double x)
Set center x-coordinate.
- VEXTERNC void `MGparm_setCenterY` (`MGparm` *thee, double y)
Set center y-coordinate.
- VEXTERNC void `MGparm_setCenterZ` (`MGparm` *thee, double z)
Set center z-coordinate.
- VEXTERNC double `MGparm_getCenterX` (`MGparm` *thee)
Get center x-coordinate.
- VEXTERNC double `MGparm_getCenterY` (`MGparm` *thee)
Get center y-coordinate.
- VEXTERNC double `MGparm_getCenterZ` (`MGparm` *thee)
Get center z-coordinate.
- VEXTERNC `MGparm` * `MGparm_ctor` (`MGparm_CalcType` type)
Construct MGparm object.
- VEXTERNC `Vrc_Codes` `MGparm_ctor2` (`MGparm` *thee, `MGparm_CalcType` type)
FORTTRAN stub to construct MGparm object.
- VEXTERNC void `MGparm_dtor` (`MGparm` **thee)
Object destructor.
- VEXTERNC void `MGparm_dtor2` (`MGparm` *thee)
FORTTRAN stub for object destructor.
- VEXTERNC `Vrc_Codes` `MGparm_check` (`MGparm` *thee)

Consistency check for parameter values stored in object.

- VEXTERNC void [MGparm_copy](#) ([MGparm](#) *thee, [MGparm](#) *parm)

Copy MGparm object into thee.

- VEXTERNC Vrc_Codes [MGparm_parseToken](#) ([MGparm](#) *thee, char tok[VMAX_BUFSIZE], Vio *sock)

Parse an MG keyword from an input file.

7.9.1 Detailed Description

Parameter which holds useful parameters for generic multigrid calculations.

7.9.2 Typedef Documentation

7.9.2.1 MGparm_CalcType

```
typedef enum eMGparm_CalcType MGparm_CalcType
```

Declare MGparm_CalcType type.

Definition at line 89 of file [mgparm.h](#).

7.9.2.2 MGparm_CentMeth

```
typedef enum eMGparm_CentMeth MGparm_CentMeth
```

Declare MGparm_CentMeth type.

Definition at line 105 of file [mgparm.h](#).

7.9.3 Enumeration Type Documentation

7.9.3.1 eMGparm_CalcType

```
enum eMGparm_CalcType
```

Calculation type.

Enumerator

MCT_MANUAL	mg-manual
MCT_AUTO	mg-auto
MCT_PARALLEL	mg-para
MCT_DUMMY	mg-dummy
MCT_NONE	unspecified

Definition at line 77 of file [mgparm.h](#).

7.9.3.2 eMGparm_CentMeth

```
enum eMGparm_CentMeth
```

Centering method.

Enumerator

MCM_POINT	Center on a point
MCM_MOLECULE	Center on a molecule
MCM_FOCUS	Determined by focusing

Definition at line 95 of file [mgparm.h](#).

7.9.4 Function Documentation

7.9.4.1 APOLparm_parseToken()

```
VEEXTERNC Vrc_Codes APOLparm_parseToken (
    APOLparm * thee,
    char tok[VMAX_BUFSIZE],
    Vio * sock )
```

Parse an MG keyword from an input file.

Author

David Gohara

Parameters

<i>thee</i>	MGparm object
<i>tok</i>	Token to parse
<i>sock</i>	Stream for more tokens

Returns

Success enumeration (1 if matched and assigned; -1 if matched, but there's some sort of error (i.e., too few args); 0 if not matched)

Definition at line 577 of file [apolparm.c](#).

7.9.4.2 FEMparm_parseToken()

```
VEEXTERNC Vrc_Codes FEMparm_parseToken (
    FEMparm * thee,
    char tok[VMAX_BUFSIZE],
    Vio * sock )
```

Parse an MG keyword from an input file.

Author

Nathan Baker

Parameters

<i>thee</i>	MGparm object
<i>tok</i>	Token to parse
<i>sock</i>	Stream for more tokens

Returns

VRC_SUCCESS if matched and assigned; VRC_FAILURE if matched, but there's some sort of error (i.e., too few args); VRC_WARNING if not matched

Definition at line 431 of file [femparm.c](#).

7.9.4.3 MGparm_check()

```
VEEXTERNC Vrc_Codes MGparm_check (
    MGparm * thee )
```

Consistency check for parameter values stored in object.

Author

Nathan Baker

Parameters

<i>thee</i>	MGparm object
-------------	---------------

Returns

Success enumeration

Definition at line 185 of file [mgparm.c](#).

7.9.4.4 MGparm_copy()

```
VEXTERNC void MGparm_copy (  
    MGparm * thee,  
    MGparm * parm )
```

Copy MGparm object into thee.

Author

Nathan Baker and Todd Dolinsky

Parameters

<i>thee</i>	MGparm object (target for copy)
<i>parm</i>	MGparm object (source for copy)

Definition at line 341 of file [mgparm.c](#).

7.9.4.5 MGparm_ctor()

```
VEXTERNC MGparm * MGparm_ctor (  
    MGparm_CalcType type )
```

Construct MGparm object.

Author

Nathan Baker

Parameters

<i>type</i>	Type of MG calculation
-------------	------------------------

Returns

Newly allocated and initialized MGparm object

Definition at line 114 of file [mgparm.c](#).

7.9.4.6 MGparm_ctor2()

```
VEXTERNC Vrc_Codes MGparm_ctor2 (  
    MGparm * thee,  
    MGparm_CalcType type )
```

FORTTRAN stub to construct MGparm object.

Author

Nathan Baker and Todd Dolinsky

Parameters

<i>thee</i>	Space for MGparm object
<i>type</i>	Type of MG calculation

Returns

Success enumeration

Definition at line 125 of file [mgparm.c](#).

7.9.4.7 MGparm_dtor()

```
VEXTERNC void MGparm_dtor (  
    MGparm ** thee )
```

Object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to memory location of MGparm object
-------------	---

Definition at line 175 of file [mgparm.c](#).

7.9.4.8 MGparm_dtor2()

```
VEXTERNC void MGparm_dtor2 (  
    MGparm * thee )
```

FORTTRAN stub for object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to MGparm object
-------------	--------------------------

Definition at line 183 of file [mgparm.c](#).

7.9.4.9 MGparm_getCenterX()

```
VEXTERNC double MGparm_getCenterX (
    MGparm * thee )
```

Get center x-coordinate.

Author

Nathan Baker

Parameters

<i>thee</i>	MGparm object
-------------	---------------

Returns

x-coordinate

Definition at line 77 of file [mgparm.c](#).

7.9.4.10 MGparm_getCenterY()

```
VEXTERNC double MGparm_getCenterY (
    MGparm * thee )
```

Get center y-coordinate.

Author

Nathan Baker

Parameters

<i>thee</i>	MGparm object
-------------	---------------

Returns

y-coordinate

Definition at line 81 of file [mgparm.c](#).

7.9.4.11 MGparm_getCenterZ()

```
VEXTERNC double MGparm_getCenterZ (
    MGparm * thee )
```

Get center z-coordinate.

Author

Nathan Baker

Parameters

<i>thee</i>	MGparm object
-------------	---------------

Returns

z-coordinate

Definition at line 85 of file [mgparm.c](#).

7.9.4.12 MGparm_getHx()

```
VEXTERNC double MGparm_getHx (  
    MGparm * thee )
```

Get grid spacing in x direction (Å)

Author

Nathan Baker

Parameters

<i>thee</i>	MGparm object
-------------	---------------

Returns

Grid spacing in the x direction

Definition at line 101 of file [mgparm.c](#).

7.9.4.13 MGparm_getHy()

```
VEXTERNC double MGparm_getHy (  
    MGparm * thee )
```

Get grid spacing in y direction (Å)

Author

Nathan Baker

Parameters

<i>thee</i>	MGparm object
-------------	---------------

Returns

Grid spacing in the y direction

Definition at line 105 of file [mgparm.c](#).

7.9.4.14 MGparm_getHz()

```
VEXTERNC double MGparm_getHz (  
    MGparm * thee )
```

Get grid spacing in z direction (Å)

Author

Nathan Baker

Parameters

<i>thee</i>	MGparm object
-------------	---------------

Returns

Grid spacing in the z direction

Definition at line 109 of file [mgparm.c](#).

7.9.4.15 MGparm_getNx()

```
VEXTERNC int MGparm_getNx (  
    MGparm * thee )
```

Get number of grid points in x direction.

Author

Nathan Baker

Parameters

<i>thee</i>	MGparm object
-------------	---------------

Returns

Number of grid points in the x direction

Definition at line 89 of file [mgparm.c](#).

7.9.4.16 MGparm_getNy()

```
VEXTERNC int MGparm_getNy (  
    MGparm * thee )
```

Get number of grid points in y direction.

Author

Nathan Baker

Parameters

<i>thee</i>	MGparm object
-------------	---------------

Returns

Number of grid points in the y direction

Definition at line 93 of file [mgparm.c](#).

7.9.4.17 MGparm_getNz()

```
VEXTERNC int MGparm_getNz (  
    MGparm * thee )
```

Get number of grid points in z direction.

Author

Nathan Baker

Parameters

<i>thee</i>	MGparm object
-------------	---------------

Returns

Number of grid points in the z direction

Definition at line 97 of file [mgparm.c](#).

7.9.4.18 MGparm_parseToken()

```
VEXTERNC Vrc_Codes MGparm_parseToken (  
    MGparm * thee,  
    char tok[VMAX_BUFSIZE],  
    Vio * sock )
```

Parse an MG keyword from an input file.

Author

Nathan Baker and Todd Dolinsky

Parameters

<i>thee</i>	MGparm object
<i>tok</i>	Token to parse
<i>sock</i>	Stream for more tokens

Returns

Success enumeration (1 if matched and assigned; -1 if matched, but there's some sort of error (i.e., too few args); 0 if not matched)

Definition at line 919 of file [mgparm.c](#).

7.9.4.19 MGparm_setCenterX()

```
VEXTERNC void MGparm_setCenterX (  
    MGparm * thee,  
    double x )
```

Set center x-coordinate.

Author

Nathan Baker

Parameters

<i>thee</i>	MGparm object
<i>x</i>	x-coordinate

Definition at line 65 of file [mgparm.c](#).

7.9.4.20 MGparm_setCenterY()

```
VEXTERNC void MGparm_setCenterY (
    MGparm * thee,
    double y )
```

Set center y-coordinate.

Author

Nathan Baker

Parameters

<i>thee</i>	MGparm object
<i>y</i>	y-coordinate

Definition at line 69 of file [mgparm.c](#).

7.9.4.21 MGparm_setCenterZ()

```
VEXTERNC void MGparm_setCenterZ (
    MGparm * thee,
    double z )
```

Set center z-coordinate.

Author

Nathan Baker

Parameters

<i>thee</i>	MGparm object
<i>z</i>	z-coordinate

Definition at line 73 of file [mgparm.c](#).

7.10 NOsh class

Class for parsing for fixed format input files.

Files

- file [nosh.c](#)
Class NOsh methods.
- file [nosh.h](#)
Contains declarations for class NOsh.

Data Structures

- struct [sNOsh_calc](#)
Calculation class for use when parsing fixed format input files.

- struct `sNOsh`

Class for parsing fixed format input files.

Macros

- #define `NOSH_MAXMOL` 20
Maximum number of molecules in a run.
- #define `NOSH_MAXCALC` 20
Maximum number of calculations in a run.
- #define `NOSH_MAXPRINT` 20
Maximum number of PRINT statements in a run.
- #define `NOSH_MAXPOP` 20
Maximum number of operations in a PRINT statement.

Typedefs

- typedef enum `eNOsh_MolFormat` `NOsh_MolFormat`
Declare NOsh_MolFormat type.
- typedef enum `eNOsh_CalcType` `NOsh_CalcType`
Declare NOsh_CalcType type.
- typedef enum `eNOsh_ParmFormat` `NOsh_ParmFormat`
Declare NOsh_ParmFormat type.
- typedef enum `eNOsh_PrintType` `NOsh_PrintType`
Declare NOsh_PrintType type.
- typedef struct `sNOsh` `NOsh`
Declaration of the NOsh class as the NOsh structure.

Enumerations

- enum `eNOsh_MolFormat` { `NMF_PQR` =0 , `NMF_PDB` =1 , `NMF_XML` =2 }
Molecule file format types.
- enum `eNOsh_CalcType` {
 `NCT_MG` =0 , `NCT_FEM` =1 , `NCT_APOL` =2 , `NCT_BEM` =3 ,
 `NCT_GEOFLOW` =4 , `NCT_PBAM` =5 , `NCT_PBSAM` =6 }
NOsh calculation types.
- enum `eNOsh_ParmFormat` { `NPF_FLAT` =0 , `NPF_XML` =1 }
Parameter file format types.
- enum `eNOsh_PrintType` {
 `NPT_ENERGY` =0 , `NPT_FORCE` =1 , `NPT_ELECENERGY` , `NPT_ELECFORCE` ,
 `NPT_APOLENERGY` , `NPT_APOLFORCE` }
NOsh print types.

Functions

- VEXTERNC char * `NOsh_getMolpath` (`NOsh` *thee, int imol)
Returns path to specified molecule.
- VEXTERNC char * `NOsh_getDielXpath` (`NOsh` *thee, int imap)
Returns path to specified x-shifted dielectric map.
- VEXTERNC char * `NOsh_getDielYpath` (`NOsh` *thee, int imap)
Returns path to specified y-shifted dielectric map.

- VEXTERNC char * [NOsh_getDielZpath](#) (NOsh *thee, int imap)
Returns path to specified z-shifted dielectric map.
- VEXTERNC char * [NOsh_getKappapath](#) (NOsh *thee, int imap)
Returns path to specified kappa map.
- VEXTERNC char * [NOsh_getPotpath](#) (NOsh *thee, int imap)
Returns path to specified potential map.
- VEXTERNC char * [NOsh_getChargepath](#) (NOsh *thee, int imap)
Returns path to specified charge distribution map.
- VEXTERNC [NOsh_calc](#) * [NOsh_getCalc](#) (NOsh *thee, int icalc)
Returns specified calculation object.
- VEXTERNC int [NOsh_getDielfmt](#) (NOsh *thee, int imap)
Returns format of specified dielectric map.
- VEXTERNC int [NOsh_getKappafmt](#) (NOsh *thee, int imap)
Returns format of specified kappa map.
- VEXTERNC int [NOsh_getPotfmt](#) (NOsh *thee, int imap)
Returns format of specified potential map.
- VEXTERNC int [NOsh_getChargefmt](#) (NOsh *thee, int imap)
Returns format of specified charge map.
- VEXTERNC [NOsh_PrintType](#) [NOsh_printWhat](#) (NOsh *thee, int iprint)
Return an integer ID of the observable to print (.
- VEXTERNC char * [NOsh_elecname](#) (NOsh *thee, int ielec)
Return an integer mapping of an ELEC statement to a calculation ID (.
- VEXTERNC int [NOsh_elec2calc](#) (NOsh *thee, int icalc)
Return the name of an elec statement.
- VEXTERNC int [NOsh_apol2calc](#) (NOsh *thee, int icalc)
Return the name of an apol statement.
- VEXTERNC int [NOsh_printNarg](#) (NOsh *thee, int iprint)
Return number of arguments to PRINT statement (.
- VEXTERNC int [NOsh_printOp](#) (NOsh *thee, int iprint, int iarg)
Return integer ID for specified operation (.
- VEXTERNC int [NOsh_printCalc](#) (NOsh *thee, int iprint, int iarg)
Return calculation ID for specified PRINT statement (.
- VEXTERNC [NOsh](#) * [NOsh_ctor](#) (int rank, int size)
Construct NOsh.
- VEXTERNC [NOsh_calc](#) * [NOsh_calc_ctor](#) (NOsh_CalcType calcType)
Construct NOsh_calc.
- VEXTERNC int [NOsh_calc_copy](#) (NOsh_calc *thee, [NOsh_calc](#) *source)
Copy NOsh_calc object into thee.
- VEXTERNC void [NOsh_calc_dtor](#) (NOsh_calc **thee)
Object destructor.
- VEXTERNC int [NOsh_ctor2](#) (NOsh *thee, int rank, int size)
FORTTRAN stub to construct NOsh.
- VEXTERNC void [NOsh_dtor](#) (NOsh **thee)
Object destructor.
- VEXTERNC void [NOsh_dtor2](#) (NOsh *thee)
FORTTRAN stub for object destructor.
- VEXTERNC int [NOsh_parseInput](#) (NOsh *thee, Vio *sock)

Parse an input file from a socket.

- VEXTERNC int [NOsh_parseInputFile](#) (NOsh *thee, char *filename)

Parse an input file only from a file.

- VEXTERNC int [NOsh_setupElecCalc](#) (NOsh *thee, Valist *alist[NOSH_MAXMOL])

Setup the series of electrostatics calculations.

- VEXTERNC int [NOsh_setupApolCalc](#) (NOsh *thee, Valist *alist[NOSH_MAXMOL])

Setup the series of non-polar calculations.

7.10.1 Detailed Description

Class for parsing for fixed format input files.

7.10.2 Macro Definition Documentation

7.10.2.1 NOSH_MAXCALC

```
#define NOSH_MAXCALC 20
```

Maximum number of calculations in a run.

Definition at line 87 of file [nosh.h](#).

7.10.2.2 NOSH_MAXMOL

```
#define NOSH_MAXMOL 20
```

Maximum number of molecules in a run.

Definition at line 83 of file [nosh.h](#).

7.10.2.3 NOSH_MAXPOP

```
#define NOSH_MAXPOP 20
```

Maximum number of operations in a PRINT statement.

Definition at line 95 of file [nosh.h](#).

7.10.2.4 NOSH_MAXPRINT

```
#define NOSH_MAXPRINT 20
```

Maximum number of PRINT statements in a run.

Definition at line 91 of file [nosh.h](#).

7.10.3 Typedef Documentation

7.10.3.1 NOsh

```
typedef struct sNOsh NOsh
```

Declaration of the NOsh class as the NOsh structure.

Definition at line 277 of file [nosh.h](#).

7.10.3.2 NOsh_CalcType

```
typedef enum eNOsh_CalcType NOsh_CalcType
```

Declare NOsh_CalcType type.

Definition at line 131 of file [nosh.h](#).

7.10.3.3 NOsh_MolFormat

```
typedef enum eNOsh_MolFormat NOsh_MolFormat
```

Declare NOsh_MolFormat type.

Definition at line 111 of file [nosh.h](#).

7.10.3.4 NOsh_ParmFormat

```
typedef enum eNOsh_ParmFormat NOsh_ParmFormat
```

Declare NOsh_ParmFormat type.

Definition at line 146 of file [nosh.h](#).

7.10.3.5 NOsh_PrintType

```
typedef enum eNOsh_PrintType NOsh_PrintType
```

Declare NOsh_PrintType type.

Definition at line 165 of file [nosh.h](#).

7.10.4 Enumeration Type Documentation

7.10.4.1 eNOsh_CalcType

```
enum eNOsh_CalcType
```

NOsh calculation types.

Enumerator

NCT_MG	Multigrid
NCT_FEM	Finite element
NCT_APOL	non-polar
NCT_BEM	Boundary element (TABI)
NCT_GEOFLOW	Geometric flow
NCT_PBAM	Analytical Poisson-Boltzmann Solver
NCT_PBSAM	Semi-Analytical Poisson-Boltzmann Solver

Definition at line 117 of file [nosh.h](#).

7.10.4.2 eNOsh_MolFormat

```
enum eNOsh_MolFormat
```

Molecule file format types.

Enumerator

NMF_PQR	PQR format
NMF_PDB	PDB format
NMF_XML	XML format

Definition at line 101 of file [nosh.h](#).

7.10.4.3 eNOsh_ParmFormat

```
enum eNOsh_ParmFormat
```

Parameter file format types.

Enumerator

NPF_FLAT	Flat-file format
NPF_XML	XML format

Definition at line 137 of file [nosh.h](#).

7.10.4.4 eNOsh_PrintType

enum [eNOsh_PrintType](#)

NOsh print types.

Enumerator

NPT_ENERGY	Energy (deprecated)
NPT_FORCE	Force (deprecated)
NPT_ELECENERGY	Elec Energy
NPT_ELECFORCE	Elec Force
NPT_APOLENERGY	Apol Energy
NPT_APOLFORCE	Apol Force

Definition at line 152 of file [nosh.h](#).

7.10.5 Function Documentation

7.10.5.1 NOsh_apol2calc()

```

VEXTERNC int NOsh_apol2calc (
    NOsh * thee,
    int icalc )

```

Return the name of an apol statement.

Author

David Gohara

Parameters

<i>thee</i>	NOsh object to use
<i>icalc</i>	ID of CALC statement

Returns

The name (if present) of an APOL statement

Definition at line 282 of file [nosh.c](#).

7.10.5.2 NOsh_calc_copy()

```

VEXTERNC int NOsh_calc_copy (
    NOsh_calc * thee,
    NOsh_calc * source )

```

Copy NOsh_calc object into thee.

Author

Nathan Baker

Parameters

<i>thee</i>	Target object
<i>source</i>	Source object

Definition at line [467](#) of file [nosh.c](#).

7.10.5.3 NOsh_calc_ctor()

```
VEXTERNC NOsh_calc * NOsh_calc_ctor (
    NOsh_CalcType calcType )
```

Construct NOsh_calc.

Author

Nathan Baker

Parameters

<i>calcType</i>	Calculation type
-----------------	------------------

Returns

Newly allocated and initialized NOsh object

Definition at line [374](#) of file [nosh.c](#).

7.10.5.4 NOsh_calc_dtor()

```
VEXTERNC void NOsh_calc_dtor (
    NOsh_calc ** thee )
```

Object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to memory location of NOsh_calc object
-------------	--

Definition at line [423](#) of file [nosh.c](#).

7.10.5.5 NOsh_ctor()

```
VEXTERNC NOsh * NOsh_ctor (
    int rank,
    int size )
```

Construct NOsh.

Author

Nathan Baker

Parameters

<i>rank</i>	Rank of current processor in parallel calculation (0 if not parallel)
<i>size</i>	Number of processors in parallel calculation (1 if not parallel)

Returns

Newly allocated and initialized NOsh object

Definition at line 308 of file [nosh.c](#).**7.10.5.6 NOsh_ctor2()**

```
VEXTERNC int NOsh_ctor2 (  
    NOsh * thee,  
    int rank,  
    int size )
```

FORTRAN stub to construct NOsh.

Author

Nathan Baker

Parameters

<i>thee</i>	Space for NOsh objet
<i>rank</i>	Rank of current processor in parallel calculation (0 if not parallel)
<i>size</i>	Number of processors in parallel calculation (1 if not parallel)

Returns

1 if successful, 0 otherwise

Definition at line 319 of file [nosh.c](#).**7.10.5.7 NOsh_dtor()**

```
VEXTERNC void NOsh_dtor (  
    NOsh ** thee )
```

Object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to memory location of NOsh object
-------------	---

Definition at line 354 of file [nosh.c](#).

7.10.5.8 NOsh_dtor2()

```
VEXTERNC void NOsh_dtor2 (
    NOsh * thee )
```

FORTTRAN stub for object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to NOsh object
-------------	------------------------

Definition at line 362 of file [nosh.c](#).

7.10.5.9 NOsh_elec2calc()

```
VEXTERNC int NOsh_elec2calc (
    NOsh * thee,
    int icalc )
```

Return the name of an elec statement.

Author

Todd Dolinsky

Parameters

<i>thee</i>	NOsh object to use
<i>icalc</i>	ID of CALC statement

Returns

The name (if present) of an ELEC statement

Definition at line 276 of file [nosh.c](#).

7.10.5.10 NOsh_elecname()

```
VEXTERNC char * NOsh_elecname (
    NOsh * thee,
    int ielec )
```

Return an integer mapping of an ELEC statement to a calculation ID (.

See also

[elec2calc\(\)](#)

Author

Nathan Baker

Parameters

<i>thee</i>	NOsh object to use
<i>ielec</i>	ID of ELEC statement

Returns

An integer mapping of an ELEC statement to a calculation ID (

See also

elec2calc)

Definition at line 288 of file [nosh.c](#).

7.10.5.11 NOsh_getCalc()

```
VEXTERNC NOsh_calc * NOsh_getCalc (
    NOsh * thee,
    int icalc )
```

Returns specified calculation object.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to NOsh object
<i>icalc</i>	Calculation ID of interest

Returns

Pointer to specified calculation object

Definition at line 235 of file [nosh.c](#).

7.10.5.12 NOsh_getChargefmt()

```
VEXTERNC int NOsh_getChargefmt (
    NOsh * thee,
    int imap )
```

Returns format of specified charge map.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to NOsh object
<i>imap</i>	Calculation ID of interest

Returns

Format of charge map

Definition at line 255 of file [nosh.c](#).

7.10.5.13 NOsh_getChargepath()

```
EXTERNC char * NOsh_getChargepath (
    NOsh * thee,
    int imap )
```

Returns path to specified charge distribution map.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to NOsh object
<i>imap</i>	Map ID of interest

Returns

Path string

Definition at line 230 of file [nosh.c](#).

7.10.5.14 NOsh_getDielFmt()

```
EXTERNC int NOsh_getDielFmt (
    NOsh * thee,
    int imap )
```

Returns format of specified dielectric map.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to NOsh object
<i>imap</i>	Calculation ID of interest

Returns

Format of dielectric map

Definition at line 240 of file [nosh.c](#).

7.10.5.15 NOsh_getDielXpath()

```
EXTERNC char * NOsh_getDielXpath (
    NOsh * thee,
    int imap )
```

Returns path to specified x-shifted dielectric map.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to NOsh object
<i>imap</i>	Map ID of interest

Returns

Path string

Definition at line 205 of file [nosh.c](#).**7.10.5.16 NOsh_getDielYpath()**

```
VEXTERNC char * NOsh_getDielYpath (
    NOsh * thee,
    int imap )
```

Returns path to specified y-shifted dielectric map.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to NOsh object
<i>imap</i>	Map ID of interest

Returns

Path string

Definition at line 210 of file [nosh.c](#).**7.10.5.17 NOsh_getDielZpath()**

```
VEXTERNC char * NOsh_getDielZpath (
    NOsh * thee,
    int imap )
```

Returns path to specified z-shifted dielectric map.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to NOsh object
<i>imap</i>	Map ID of interest

Returns

Path string

Definition at line 215 of file [nosh.c](#).

7.10.5.18 NOsh_getKappafmt()

```
EXTERNC int NOsh_getKappafmt (
    NOsh * thee,
    int imap )
```

Returns format of specified kappa map.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to NOsh object
<i>imap</i>	Calculation ID of interest

Returns

Format of kappa map

Definition at line 245 of file [nosh.c](#).

7.10.5.19 NOsh_getKappapath()

```
EXTERNC char * NOsh_getKappapath (
    NOsh * thee,
    int imap )
```

Returns path to specified kappa map.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to NOsh object
<i>imap</i>	Map ID of interest

Returns

Path string

Definition at line 220 of file [nosh.c](#).

7.10.5.20 NOsh_getMolpath()

```
EXTERNC char * NOsh_getMolpath (
    NOsh * thee,
    int imol )
```

Returns path to specified molecule.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to NOsh object
<i>imol</i>	Molecule ID of interest

Returns

Path string

Definition at line 200 of file [nosh.c](#).**7.10.5.21 NOsh_getPotfmt()**

```
VEXTERNC int NOsh_getPotfmt (  
    NOsh * thee,  
    int imap )
```

Returns format of specified potential map.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to NOsh object
<i>imap</i>	Calculation ID of interest

Returns

Format of potential map

Definition at line 250 of file [nosh.c](#).**7.10.5.22 NOsh_getPotpath()**

```
VEXTERNC char * NOsh_getPotpath (  
    NOsh * thee,  
    int imap )
```

Returns path to specified potential map.

Author

David Gohara

Parameters

<i>thee</i>	Pointer to NOsh object
<i>imap</i>	Map ID of interest

Returns

Path string

Definition at line 225 of file [nosh.c](#).

7.10.5.23 NOsh_parseInput()

```
VEXTERNC int NOsh_parseInput (
    NOsh * thee,
    Vio * sock )
```

Parse an input file from a socket.

Note

Should be called before NOsh_setupCalc

Author

Nathan Baker and Todd Dolinsky

Parameters

<i>thee</i>	Pointer to NOsh object
<i>sock</i>	Stream of tokens to parse

Returns

1 if successful, 0 otherwise

Definition at line 513 of file [nosh.c](#).

7.10.5.24 NOsh_parseInputFile()

```
VEXTERNC int NOsh_parseInputFile (
    NOsh * thee,
    char * filename )
```

Parse an input file only from a file.

Note

Included for SWIG wrapper compatibility

Should be called before NOsh_setupCalc

Author

Nathan Baker and Todd Dolinsky

Parameters

<i>thee</i>	Pointer to NOsh object
<i>filename</i>	Name/path of readable file

Returns

1 if successful, 0 otherwise

Definition at line 498 of file [nosh.c](#).

7.10.5.25 NOsh_printCalc()

```
VEXTERNC int NOsh_printCalc (
    NOsh * thee,
    int iprint,
    int iarg )
```

Return calculation ID for specified PRINT statement (.

See also

printcalc)

Author

Nathan Baker

Parameters

<i>thee</i>	NOsh object to use
<i>iprint</i>	ID of PRINT statement
<i>iarg</i>	ID of operation in PRINT statement

Returns

Calculation ID for specified PRINT statement (

See also

printcalc)

Definition at line 301 of file [nosh.c](#).

7.10.5.26 NOsh_printNarg()

```
VEXTERNC int NOsh_printNarg (
    NOsh * thee,
    int iprint )
```

Return number of arguments to PRINT statement (.

See also

printrnarg)

Author

Nathan Baker

Parameters

<i>thee</i>	NOsh object to use
<i>iprint</i>	ID of PRINT statement

Returns

Number of arguments to PRINT statement (

See also

printrarg)

Definition at line 270 of file [nosh.c](#).

7.10.5.27 NOsh_printOp()

```
EXTERNC int NOsh_printOp (  
    NOsh * thee,  
    int iprint,  
    int iarg )
```

Return integer ID for specified operation (.

See also

printop)

Author

Nathan Baker

Parameters

<i>thee</i>	NOsh object to use
<i>iprint</i>	ID of PRINT statement
<i>iarg</i>	ID of operation in PRINT statement

Returns

Integer ID for specified operation (

See also

printop)

Definition at line 294 of file [nosh.c](#).

7.10.5.28 NOsh_printWhat()

```
EXTERNC NOsh_PrintType NOsh_printWhat (  
    NOsh * thee,  
    int iprint )
```

Return an integer ID of the observable to print (.

See also

printwhat)

Author

Nathan Baker

Parameters

<i>thee</i>	NOsh object to use
<i>iprint</i>	ID of PRINT statement

Returns

An integer ID of the observable to print (

See also

printwhat)

Definition at line 264 of file [nosh.c](#).

7.10.5.29 NOsh_setupApolCalc()

```
VEXTERNC int NOsh_setupApolCalc (
    NOsh * thee,
    Valist * alist[NOSH_MAXMOL] )
```

Setup the series of non-polar calculations.

Note

Should be called after NOsh_parseInput*

Author

Nathan Baker and Todd Dolinsky

Parameters

<i>thee</i>	Pointer to NOsh object
<i>alist</i>	Array of pointers to Valist objects (molecules used to center mesh);

Returns

1 if successful, 0 otherwise

Parameters

<i>thee</i>	NOsh object
<i>alist</i>	Atom list for calculation

Definition at line 1469 of file [nosh.c](#).

7.10.5.30 NOsh_setupElecCalc()

```
VEXTERNC int NOsh_setupElecCalc (
    NOsh * thee,
    Valist * alist[NOSH_MAXMOL] )
```

Setup the series of electrostatics calculations.

Note

Should be called after NOsh_parseInput*

Author

Nathan Baker and Todd Dolinsky

Parameters

<i>thee</i>	Pointer to NOsh object
<i>alist</i>	Array of pointers to Valist objects (molecules used to center mesh);

Returns

1 if successful, 0 otherwise

Parameters

<i>thee</i>	NOsh object
<i>alist</i>	Atom list for calculation

Definition at line 1374 of file [nosh.c](#).

7.11 PBAMparm class

Parameter which holds useful parameters for Poisson-boltzmann analytical method calculations.

Files

- file [pbamparm.c](#)
Class PBAMparm methods.
- file [pbamparm.h](#)
Contains declarations for class PBAMparm.

Data Structures

- struct [sPBAMparm](#)
Parameter structure for PBAM-specific variables from input files.

Macros

- `#define` [CHR_MAXLEN](#) 1000
Number of things that can be written out in a single calculation.

Typedefs

- typedef enum [ePBAMparm_CalcType](#) [PBAMparm_CalcType](#)
Declare PBAMparm_CalcType type.
- typedef struct [sPBAMparm](#) [PBAMparm](#)
Parameter structure for PBAM-specific variables from input files.

Enumerations

- enum `ePBAMparm_CalcType` { `PBAMCT_AUTO` =1 }
Calculation type.

Functions

- VEXTERNC `PBAMparm * PBAMparm_ctor` (`PBAMparm_CalcType` type)
Construct PBAMparm object.
- VEXTERNC `Vrc_Codes PBAMparm_ctor2` (`PBAMparm *thee`, `PBAMparm_CalcType` type)
FORTRAN stub to construct PBAMparm object ????????!!!!!!
- VEXTERNC void `PBAMparm_dtor` (`PBAMparm **thee`)
Object destructor.
- VEXTERNC void `PBAMparm_dtor2` (`PBAMparm *thee`)
FORTRAN stub for object destructor ????????!!!!!!
- VEXTERNC `Vrc_Codes PBAMparm_check` (`PBAMparm *thee`)
Consistency check for parameter values stored in object.
- VEXTERNC `Vrc_Codes PBAMparm_parseToken` (`PBAMparm *thee`, char tok[VMAX_BUFSIZE], `Vio *sock`)
Parse an MG keyword from an input file.
- VEXTERNC void `PBAMparm_copy` (`PBAMparm *thee`, `PBAMparm *parm`)
copy PBAMparm object into thee.
- VPRIVATE `Vrc_Codes PBAMparm_parseSalt` (`PBAMparm *thee`, `Vio *sock`)
Find salt conc and save it as a structure variable.
- VPRIVATE `Vrc_Codes PBAMparm_parseRunType` (`PBAMparm *thee`, `Vio *sock`)
Find runType and save it as a structure variable.
- VPRIVATE `Vrc_Codes PBAMparm_parseRunName` (`PBAMparm *thee`, `Vio *sock`)
Find runName and save it as a structure variable.
- VPRIVATE `Vrc_Codes PBAMparm_parseRandorient` (`PBAMparm *thee`, `Vio *sock`)
Find randomorientation flag and save it as a boolean.
- VPRIVATE `Vrc_Codes PBAMparm_parsePBCS` (`PBAMparm *thee`, `Vio *sock`)
Find PBC flag and save the type and the boxlength.
- VPRIVATE `Vrc_Codes PBAMparm_parseUnits` (`PBAMparm *thee`, `Vio *sock`)
Find units flag and save units.
- VPRIVATE `Vrc_Codes PBAMparm_parse3Dmap` (`PBAMparm *thee`, `Vio *sock`)
Find 3D map filename and save it.
- VPRIVATE `Vrc_Codes PBAMparm_parseGrid2D` (`PBAMparm *thee`, `Vio *sock`)
Find 2D grid filename and save it.
- VPRIVATE `Vrc_Codes PBAMparm_parseDX` (`PBAMparm *thee`, `Vio *sock`)
Find DX filename and save it.
- VPRIVATE `Vrc_Codes PBAMparm_parseGridPts` (`PBAMparm *thee`, `Vio *sock`)
Find Grid points and save them.
- VPRIVATE `Vrc_Codes PBAMparm_parseTermcombine` (`PBAMparm *thee`, `Vio *sock`)
Find Termination logic and save it.
- VPRIVATE `Vrc_Codes PBAMparm_parseDiff` (`PBAMparm *thee`, `Vio *sock`)
Find diffusion coeffs for each molecule and save them.
- VPRIVATE `Vrc_Codes PBAMparm_parseXYZ` (`PBAMparm *thee`, `Vio *sock`)
Find xyz files for each molecule for each traj and save them.

7.11.1 Detailed Description

Parameter which holds useful parameters for Poisson-boltzmann analytical method calculations.

7.11.2 Macro Definition Documentation

7.11.2.1 CHR_MAXLEN

```
#define CHR_MAXLEN 1000
```

Number of things that can be written out in a single calculation.

Definition at line 76 of file [pbamparm.h](#).

7.11.3 Typedef Documentation

7.11.3.1 PBAMparm

```
typedef struct sPBAMparm PBAMparm
```

Parameter structure for PBAM-specific variables from input files.

Author

Andrew Stevens, Kyle Monson

Note

If you add/delete/change something in this class, the member functions – especially PBAMparm_copy – must be modified accordingly

7.11.3.2 PBAMparm_CalcType

```
typedef enum ePBAMparm_CalcType PBAMparm_CalcType
```

Declare PBAMparm_CalcType type.

Definition at line 95 of file [pbamparm.h](#).

7.11.4 Enumeration Type Documentation

7.11.4.1 ePBAMparm_CalcType

```
enum ePBAMparm_CalcType
```

Calculation type.

Enumerator

PBAMCT_AUTO	PBAM-auto
-------------	-----------

Definition at line 84 of file [pbamparm.h](#).

7.11.5 Function Documentation

7.11.5.1 PBAMparm_check()

```
VEXTERNC Vrc_Codes PBAMparm_check (
    PBAMparm * thee )
```

Consistency check for parameter values stored in object.

Author

Andrew Stevens, Kyle Monson

Parameters

<i>thee</i>	PBAMparm object
-------------	-----------------

Returns

Success enumeration

Definition at line 132 of file [pbamparm.c](#).

7.11.5.2 PBAMparm_copy()

```
VEXTERNC void PBAMparm_copy (  
    PBAMparm * thee,  
    PBAMparm * parm )
```

copy PBAMparm object into *thee*.

Author**Parameters**

<i>thee</i>	PBAMparm object to be copied into
<i>parm</i>	PBAMparm object.

Definition at line 157 of file [pbamparm.c](#).

7.11.5.3 PBAMparm_ctor()

```
VEXTERNC PBAMparm * PBAMparm_ctor (  
    PBAMparm_CalcType type )
```

Construct PBAMparm object.

Author

Andrew Stevens, Kyle Monson

Parameters

<i>type</i>	Type of PBAM calculation
-------------	--------------------------

Returns

Newly allocated and initialized PBAMparm object

Definition at line 66 of file [pbamparm.c](#).

7.11.5.4 PBAMparm_ctor2()

```
VEXTERNC Vrc_Codes PBAMparm_ctor2 (
```

```
PBAMparm * thee,
PBAMparm_CalcType type )
```

FORTRAN stub to construct PBAMparm object ?????????!!!!!!

Author

Andrew Stevens, Kyle Monson

Parameters

<i>thee</i>	Space for PBAMparm object
<i>type</i>	Type of MG calculation

Returns

Success enumeration

Definition at line 77 of file [pbamparm.c](#).

7.11.5.5 PBAMparm_dtor()

```
VEXTERNC void PBAMparm_dtor (
    PBAMparm ** thee )
```

Object destructor.

Author

Andrew Stevens, Kyle Monson

Parameters

<i>thee</i>	Pointer to memory location of PBAMparm object
-------------	---

Definition at line 122 of file [pbamparm.c](#).

7.11.5.6 PBAMparm_dtor2()

```
VEXTERNC void PBAMparm_dtor2 (
    PBAMparm * thee )
```

FORTRAN stub for object destructor ?????????!!!!!!

Author

Andrew Stevens, Kyle Monson

Parameters

<i>thee</i>	Pointer to PBAMparm object
-------------	----------------------------

Definition at line 130 of file [pbamparm.c](#).

7.11.5.7 PBAMparm_parse3Dmap()

```
VPRIVATE Vrc_Codes PBAMparm_parse3Dmap (
```



```
PBAMparm * thee,  
Vio * sock )
```

Find 3D map filename and save it.

Author

Parameters

<i>thee</i>	PBAMparm object to be copied into
<i>sock</i>	The stream from which parameter is taken

Definition at line 371 of file [pbamparm.c](#).

7.11.5.8 PBAMparm_parseDiff()

```
VPRIVATE Vrc_Codes PBAMparm_parseDiff (  
    PBAMparm * thee,  
    Vio * sock )
```

Find diffusion coeffs for each molecule and save them.

Author

Parameters

<i>thee</i>	PBAMparm object to be copied into
<i>sock</i>	The stream from which parameter is taken

Definition at line 477 of file [pbamparm.c](#).

7.11.5.9 PBAMparm_parseDX()

```
VPRIVATE Vrc_Codes PBAMparm_parseDX (  
    PBAMparm * thee,  
    Vio * sock )
```

Find DX filename and save it.

Author

Parameters

<i>thee</i>	PBAMparm object to be copied into
<i>sock</i>	The stream from which parameter is taken

Definition at line 426 of file [pbamparm.c](#).

7.11.5.10 PBAMparm_parseGrid2D()

```
VPRIVATE Vrc_Codes PBAMparm_parseGrid2D (  

```

```

    PBAMparm * thee,
    Vio * sock )

```

Find 2D grid filename and save it.

Author

Parameters

<i>thee</i>	PBAMparm object to be copied into
<i>sock</i>	The stream from which parameter is taken

Definition at line 391 of file [pbamparm.c](#).

7.11.5.11 PBAMparm_parseGridPts()

```

VPRIVATE Vrc_Codes PBAMparm_parseGridPts (
    PBAMparm * thee,
    Vio * sock )

```

Find Grid points and save them.

Author

Parameters

<i>thee</i>	PBAMparm object to be copied into
<i>sock</i>	The stream from which parameter is taken

Definition at line 351 of file [pbamparm.c](#).

7.11.5.12 PBAMparm_parsePBCS()

```

VPRIVATE Vrc_Codes PBAMparm_parsePBCS (
    PBAMparm * thee,
    Vio * sock )

```

Find PBC flag and save the type and the boxlength.

Author

Parameters

<i>thee</i>	PBAMparm object to be copied into
<i>sock</i>	The stream from which parameter is taken

Definition at line 310 of file [pbamparm.c](#).

7.11.5.13 PBAMparm_parseRanderient()

```

VPRIVATE Vrc_Codes PBAMparm_parseRanderient (

```

```
PBAMparm * thee,  
Vio * sock )
```

Find randomorientation flag and save it as a boolean.

Author

Parameters

<i>thee</i>	PBAMparm object to be copied into
<i>sock</i>	The stream from which parameter is taken

Definition at line 304 of file [pbamparm.c](#).

7.11.5.14 PBAMparm_parseRunName()

```
VPRIVATE Vrc_Codes PBAMparm_parseRunName (  
    PBAMparm * thee,  
    Vio * sock )
```

Find runName and save it as a structure variable.

Author

Parameters

<i>thee</i>	PBAMparm object to be copied into
<i>sock</i>	The stream from which parameter is taken

Definition at line 289 of file [pbamparm.c](#).

7.11.5.15 PBAMparm_parseRunType()

```
VPRIVATE Vrc_Codes PBAMparm_parseRunType (  
    PBAMparm * thee,  
    Vio * sock )
```

Find runType and save it as a structure variable.

Author

Parameters

<i>thee</i>	PBAMparm object to be copied into
<i>sock</i>	The stream from which parameter is taken

Definition at line 271 of file [pbamparm.c](#).

7.11.5.16 PBAMparm_parseSalt()

```
VPRIVATE Vrc_Codes PBAMparm_parseSalt (  

```

```
PBAMparm * thee,  
Vio * sock )
```

Find salt conc and save it as a structure variable.

Author

Parameters

<i>thee</i>	PBAMparm object to be copied into
<i>parm</i>	The stream from which parameter is taken

Definition at line 252 of file [pbamparm.c](#).

7.11.5.17 PBAMparm_parseTermcombine()

```
VPRIVATE Vrc_Codes PBAMparm_parseTermcombine (  
    PBAMparm * thee,  
    Vio * sock )
```

Find Termination logic and save it.

Author

Parameters

<i>thee</i>	PBAMparm object to be copied into
<i>sock</i>	The stream from which parameter is taken

Definition at line 444 of file [pbamparm.c](#).

7.11.5.18 PBAMparm_parseToken()

```
VEXTERNC Vrc_Codes PBAMparm_parseToken (  
    PBAMparm * thee,  
    char tok[VMAX_BUFSIZE],  
    Vio * sock )
```

Parse an MG keyword from an input file.

Author

Andrew Stevens, Kyle Monson

Parameters

<i>thee</i>	PBAMparm object
<i>tok</i>	Token to parse
<i>sock</i>	Stream for more tokens

Returns

Success enumeration (1 if matched and assigned; -1 if matched, but there's some sort of error (i.e., too few args); 0 if not matched)

Definition at line 662 of file [pbamparm.c](#).

7.11.5.19 PBAMparm_parseUnits()

```
VPRIVATE Vrc_Codes PBAMparm_parseUnits (
    PBAMparm * thee,
    Vio * sock )
```

Find units flag and save units.

Author**Parameters**

<i>thee</i>	PBAMparm object to be copied into
<i>sock</i>	The stream from which parameter is taken

Definition at line 336 of file [pbamparm.c](#).

7.11.5.20 PBAMparm_parseXYZ()

```
VPRIVATE Vrc_Codes PBAMparm_parseXYZ (
    PBAMparm * thee,
    Vio * sock )
```

Find xyz files for each molecule for each traj and save them.

Author**Parameters**

<i>thee</i>	PBAMparm object to be copied into
<i>sock</i>	The stream from which parameter is taken

Definition at line 632 of file [pbamparm.c](#).

7.12 PBEparm class

Parameter structure for PBE variables independent of solver.

Files

- file [pbeparm.c](#)
Class PBEparm methods.
- file [pbeparm.h](#)
Contains declarations for class PBEparm.

Data Structures

- struct [sPBEparm](#)
Parameter structure for PBE variables from input files.

Macros

- #define [PBEARM_MAXWRITE](#) 20
Number of things that can be written out in a single calculation.

Typedefs

- typedef enum [ePBEparm_calcEnergy](#) [PBEparm_calcEnergy](#)
Define ePBEparm_calcEnergy enumeration as PBEparm_calcEnergy.
- typedef enum [ePBEparm_calcForce](#) [PBEparm_calcForce](#)
Define ePBEparm_calcForce enumeration as PBEparm_calcForce.
- typedef struct [sPBEparm](#) [PBEparm](#)
Declaration of the PBEparm class as the PBEparm structure.

Enumerations

- enum [ePBEparm_calcEnergy](#) { [PCE_NO](#) =0 , [PCE_TOTAL](#) =1 , [PCE_COMPS](#) =2 }
Define energy calculation enumeration.
- enum [ePBEparm_calcForce](#) { [PCF_NO](#) =0 , [PCF_TOTAL](#) =1 , [PCF_COMPS](#) =2 }
Define force calculation enumeration.

Functions

- VEXTERNC double [PBEparm_getIonCharge](#) ([PBEparm](#) *thee, int iion)
Get charge (e) of specified ion species.
- VEXTERNC double [PBEparm_getIonConc](#) ([PBEparm](#) *thee, int iion)
Get concentration (M) of specified ion species.
- VEXTERNC double [PBEparm_getIonRadius](#) ([PBEparm](#) *thee, int iion)
Get radius (A) of specified ion species.
- VEXTERNC [PBEparm](#) * [PBEparm_ctor](#) ()
Construct PBEparm object.
- VEXTERNC int [PBEparm_ctor2](#) ([PBEparm](#) *thee)
FORTTRAN stub to construct PBEparm object.
- VEXTERNC void [PBEparm_dtor](#) ([PBEparm](#) **thee)
Object destructor.
- VEXTERNC void [PBEparm_dtor2](#) ([PBEparm](#) *thee)
FORTTRAN stub for object destructor.
- VEXTERNC int [PBEparm_check](#) ([PBEparm](#) *thee)
Consistency check for parameter values stored in object.
- VEXTERNC void [PBEparm_copy](#) ([PBEparm](#) *thee, [PBEparm](#) *parm)
Copy PBEparm object into thee.
- VEXTERNC int [PBEparm_parseToken](#) ([PBEparm](#) *thee, char tok[VMAX_BUFSIZE], Vio *sock)
Parse a keyword from an input file.

7.12.1 Detailed Description

Parameter structure for PBE variables independent of solver.

7.12.2 Macro Definition Documentation

7.12.2.1 PBEPARM_MAXWRITE

```
#define PBEPARM_MAXWRITE 20
```

Number of things that can be written out in a single calculation.

Definition at line 75 of file [pbeparm.h](#).

7.12.3 Typedef Documentation

7.12.3.1 PBEparm

```
typedef struct sPBEparm PBEparm
```

Declaration of the PBEparm class as the PBEparm structure.

Definition at line 213 of file [pbeparm.h](#).

7.12.3.2 PBEparm_calcEnergy

```
typedef enum ePBEparm_calcEnergy PBEparm_calcEnergy
```

Define ePBEparm_calcEnergy enumeration as PBEparm_calcEnergy.

Definition at line 91 of file [pbeparm.h](#).

7.12.3.3 PBEparm_calcForce

```
typedef enum ePBEparm_calcForce PBEparm_calcForce
```

Define ePBEparm_calcForce enumeration as PBEparm_calcForce.

Definition at line 107 of file [pbeparm.h](#).

7.12.4 Enumeration Type Documentation

7.12.4.1 ePBEparm_calcEnergy

```
enum ePBEparm_calcEnergy
```

Define energy calculation enumeration.

Enumerator

PCE_NO	Do not perform energy calculation
PCE_TOTAL	Calculate total energy only
PCE_COMPS	Calculate per-atom energy components

Definition at line 81 of file [pbeparm.h](#).

7.12.4.2 ePBEparm_calcForce

```
enum ePBEparm_calcForce
```

Define force calculation enumeration.

Enumerator

PCF_NO	Do not perform force calculation
PCF_TOTAL	Calculate total force only

Enumerator

PCF_COMPS	Calculate per-atom force components
-----------	-------------------------------------

Definition at line 97 of file [pbeparm.h](#).

7.12.5 Function Documentation

7.12.5.1 PBEparm_check()

```
VEXTERNC int PBEparm_check (  
    PBEparm * thee )
```

Consistency check for parameter values stored in object.

Author

Nathan Baker

Returns

1 if OK, 0 otherwise

Parameters

<i>thee</i>	Object to be checked
-------------	----------------------

Definition at line 183 of file [pbeparm.c](#).

7.12.5.2 PBEparm_copy()

```
VEXTERNC void PBEparm_copy (  
    PBEparm * thee,  
    PBEparm * parm )
```

Copy PBEparm object into thee.

Author

Nathan Baker

Parameters

<i>thee</i>	Target for copy
<i>parm</i>	Source for copy

Definition at line 283 of file [pbeparm.c](#).

7.12.5.3 PBEparm_ctor()

```
VEXTERNC PBEparm * PBEparm_ctor ( )
```

Construct PBEparm object.

Author

Nathan Baker

Returns

Newly allocated and initialized PBEparm object

Definition at line 104 of file [pbeparm.c](#).

7.12.5.4 PBEparm_ctor2()

```
VEXTERNC int PBEparm_ctor2 (  
    PBEparm * thee )
```

FORTTRAN stub to construct PBEparm object.

Author

Nathan Baker

Returns

1 if succesful, 0 otherwise

Parameters

<i>thee</i>	Memory location for object
-------------	----------------------------

Definition at line 115 of file [pbeparm.c](#).

7.12.5.5 PBEparm_dtor()

```
VEXTERNC void PBEparm_dtor (  
    PBEparm ** thee )
```

Object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to memory location of object
-------------	--------------------------------------

Definition at line 173 of file [pbeparm.c](#).

7.12.5.6 PBEparm_dtor2()

```
VEXTERNC void PBEparm_dtor2 (  
    PBEparm * thee )
```

FORTTRAN stub for object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to object to be destroyed
-------------	-----------------------------------

Definition at line 181 of file [pbeparm.c](#).

7.12.5.7 PBEparm_getIonCharge()

```
VEXTERNC double PBEparm_getIonCharge (
    PBEparm * thee,
    int iion )
```

Get charge (e) of specified ion species.

Author

Nathan Baker

Returns

Charge of ion species (e)

Parameters

<i>thee</i>	PBEparm object
<i>iion</i>	Ion species ID/index

Definition at line 65 of file [pbeparm.c](#).

7.12.5.8 PBEparm_getIonConc()

```
VEXTERNC double PBEparm_getIonConc (
    PBEparm * thee,
    int iion )
```

Get concentration (M) of specified ion species.

Author

Nathan Baker

Returns

Concentration of ion species (M)

Parameters

<i>thee</i>	PBEparm object
<i>iion</i>	Ion species ID/index

Definition at line 71 of file [pbeparm.c](#).

7.12.5.9 PBEparm_getIonRadius()

```
VEXTERNC double PBEparm_getIonRadius (
    PBEparm * thee,
    int iion )
```

Get radius (A) of specified ion species.

Author

Nathan Baker

Returns

Radius of ion species (A)

Parameters

<i>thee</i>	PBEparm object
<i>iion</i>	Ion species ID/index

Definition at line 77 of file [pbeparm.c](#).**7.12.5.10 PBEparm_parseToken()**

```

VEXTERNC int PBEparm_parseToken (
    PBEparm * thee,
    char tok[VMAX_BUFSIZE],
    Vio * sock )

```

Parse a keyword from an input file.

Author

Nathan Baker

Returns

1 if matched and assigned; -1 if matched, but there's some sort of error (i.e., too few args); 0 if not matched

Parameters

<i>thee</i>	Parsing object
<i>tok</i>	Token to parse
<i>sock</i>	Socket for additional tokens

Definition at line 1215 of file [pbeparm.c](#).**7.13 PBSAMparm class**

Parameter which holds useful parameters for Poisson-boltzmann analytical method calculations.

Files

- file [pbsamparm.c](#)
Class PBSAMparm methods.
- file [pbsamparm.h](#)
Contains declarations for class PBSAMparm.

Data Structures

- struct [sPBSAMparm](#)

Parameter structure for PBSAM-specific variables from input files.

Macros

- #define `CHR_MAXLEN` 1000
Number of things that can be written out in a single calculation.

Typedefs

- typedef enum `ePBSAMparm_CalcType` `PBSAMparm_CalcType`
Declare PBSAMparm_CalcType type.
- typedef struct `sPBSAMparm` `PBSAMparm`
Parameter structure for PBSAM-specific variables from input files.

Enumerations

- enum `ePBSAMparm_CalcType` { `PBSAMCT_AUTO` =1 }
Calculation type.

Functions

- VEXTERNC `PBSAMparm *` `PBSAMparm_ctor` (`PBSAMparm_CalcType` type)
Construct PBSAMparm object.
- VEXTERNC `Vrc_Codes` `PBSAMparm_ctor2` (`PBSAMparm *`thee, `PBSAMparm_CalcType` type)
FORTTRAN stub to construct PBSAMparm object ?????????!!!!!!!
- VEXTERNC void `PBSAMparm_dtor` (`PBSAMparm *`thee)
Object destructor.
- VEXTERNC void `PBSAMparm_dtor2` (`PBSAMparm *`thee)
FORTTRAN stub for object destructor ?????????!!!!!!!
- VEXTERNC `Vrc_Codes` `PBSAMparm_check` (`PBSAMparm *`thee)
Consistency check for parameter values stored in object.
- VEXTERNC `Vrc_Codes` `PBSAMparm_parseToken` (`PBSAMparm *`thee, char tok[VMAX_BUFSIZE], `Vio *`sock)
Parse an MG keyword from an input file.
- VEXTERNC void `PBSAMparm_copy` (`PBSAMparm *`thee, `PBSAMparm *`parm)
copy PBSAMparm object into thee.
- VPRIVATE `Vrc_Codes` `PBSAMparm_parseTolsp` (`PBSAMparm *`thee, `Vio *`sock)
Find sphere tolerance for coarse-graining.
- VPRIVATE `Vrc_Codes` `PBSAMparm_parseSurf` (`PBSAMparm *`thee, `Vio *`sock)
Find vertex files for each molecule and save them.
- VPRIVATE `Vrc_Codes` `PBSAMparm_parselmat` (`PBSAMparm *`thee, `Vio *`sock)
Find IMAT files for each molecule and save them.
- VPRIVATE `Vrc_Codes` `PBSAMparm_parseExp` (`PBSAMparm *`thee, `Vio *`sock)
Find expansion files for each molecule and save them.
- VPRIVATE `Vrc_Codes` `PBSAMparm_parseMSMS` (`PBSAMparm *`thee, `Vio *`sock)
Find msms flag for if MSMS is to be run.

7.13.1 Detailed Description

Parameter which holds useful parameters for Poisson-boltzmann analytical method calculations.

7.13.2 Macro Definition Documentation

7.13.2.1 CHR_MAXLEN

```
#define CHR_MAXLEN 1000
```

Number of things that can be written out in a single calculation.

Definition at line 76 of file [pbsamparm.h](#).

7.13.3 Typedef Documentation

7.13.3.1 PBSAMparm

```
typedef struct sPBSAMparm PBSAMparm
```

Parameter structure for PBSAM-specific variables from input files.

Author

Lisa Felberg

Note

If you add/delete/change something in this class, the member functions – especially PBSAMparm_copy – must be modified accordingly

7.13.3.2 PBSAMparm_CalcType

```
typedef enum ePBSAMparm_CalcType PBSAMparm_CalcType
```

Declare PBSAMparm_CalcType type.

Definition at line 95 of file [pbsamparm.h](#).

7.13.4 Enumeration Type Documentation

7.13.4.1 ePBSAMparm_CalcType

```
enum ePBSAMparm_CalcType
```

Calculation type.

Enumerator

PBSAMCT_AUTO	PBSAM-auto
--------------	------------

Definition at line 84 of file [pbsamparm.h](#).

7.13.5 Function Documentation

7.13.5.1 PBSAMparm_check()

```
VEXTERNC Vrc_Codes PBSAMparm_check (
    PBSAMparm * thee )
```

Consistency check for parameter values stored in object.

Author

Lisa Felberg

Parameters

<i>thee</i>	PBSAMparm object
-------------	------------------

Returns

Success enumeration

Definition at line 110 of file [pbsamparm.c](#).

7.13.5.2 PBSAMparm_copy()

```
VEXTERNC void PBSAMparm_copy (
    PBSAMparm * thee,
    PBSAMparm * parm )
```

copy PBSAMparm object into thee.

Author**Parameters**

<i>thee</i>	PBSAMparm object to be copied into
<i>parm</i>	PBSAMparm object.

Definition at line 135 of file [pbsamparm.c](#).

7.13.5.3 PBSAMparm_ctor()

```
VEXTERNC PBSAMparm * PBSAMparm_ctor (
    PBSAMparm_CalcType type )
```

Construct PBSAMparm object.

Author

Lisa Felberg

Parameters

<i>type</i>	Type of PBSAM calculation
-------------	---------------------------

Returns

Newly allocated and initialized PBSAMparm object

Definition at line 66 of file [pbsamparm.c](#).

7.13.5.4 PBSAMparm_ctor2()

```
VEXTERNC Vrc_Codes PBSAMparm_ctor2 (
    PBSAMparm * thee,
    PBSAMparm_CalcType type )
```

FORTTRAN stub to construct PBSAMparm object ?????????!!!!!!

Author

Lisa Felberg

Parameters

<i>thee</i>	Space for PBSAMparm object
<i>type</i>	Type of MG calculation

Returns

Success enumeration

Definition at line 77 of file [pbsamparm.c](#).**7.13.5.5 PBSAMparm_dtor()**

```
VEXTERNC void PBSAMparm_dtor (
    PBSAMparm ** thee )
```

Object destructor.

Author

Lisa Felberg

Parameters

<i>thee</i>	Pointer to memory location of PBSAMparm object
-------------	--

Definition at line 100 of file [pbsamparm.c](#).**7.13.5.6 PBSAMparm_dtor2()**

```
VEXTERNC void PBSAMparm_dtor2 (
    PBSAMparm * thee )
```

FORTRAN stub for object destructor ??????????!!!!!!!!!!!!

Author

Lisa Felberg

Parameters

<i>thee</i>	Pointer to PBSAMparm object
-------------	-----------------------------

Definition at line 108 of file [pbsamparm.c](#).**7.13.5.7 PBSAMparm_parseExp()**

```
VPRIVATE Vrc_Codes PBSAMparm_parseExp (
    PBSAMparm * thee,
    Vio * sock )
```

Find expansion files for each molecule and save them.

Author

Parameters

<i>thee</i>	PBSAMparm object to be copied into
<i>sock</i>	The stream from which parameter is taken

Definition at line 218 of file [pbsamparm.c](#).

7.13.5.8 PBSAMparm_parseImat()

```
VPRIVATE Vrc_Codes PBSAMparm_parseImat (
    PBSAMparm * thee,
    Vio * sock )
```

Find IMAT files for each molecule and save them.

Author

Parameters

<i>thee</i>	PBSAMparm object to be copied into
<i>sock</i>	The stream from which parameter is taken

Definition at line 203 of file [pbsamparm.c](#).

7.13.5.9 PBSAMparm_parseMSMS()

```
VPRIVATE Vrc_Codes PBSAMparm_parseMSMS (
    PBSAMparm * thee,
    Vio * sock )
```

Find msms flag for if MSMS is to be run.

Author

Parameters

<i>thee</i>	PBSAMparm object to be copied into
<i>sock</i>	The stream from which parameter is taken

Definition at line 182 of file [pbsamparm.c](#).

7.13.5.10 PBSAMparm_parseSurf()

```
VPRIVATE Vrc_Codes PBSAMparm_parseSurf (
    PBSAMparm * thee,
    Vio * sock )
```

Find vertex files for each molecule and save them.

Author

Parameters

<i>thee</i>	PBSAMparm object to be copied into
<i>sock</i>	The stream from which parameter is taken

Definition at line 166 of file [pbsamparm.c](#).

7.13.5.11 PBSAMparm_parseToken()

```

VEXTERNC Vrc_Codes PBSAMparm_parseToken (
    PBSAMparm * thee,
    char tok[VMAX_BUFSIZE],
    Vio * sock )

```

Parse an MG keyword from an input file.

Author

Lisa Felberg

Parameters

<i>thee</i>	PBSAMparm object
<i>tok</i>	Token to parse
<i>sock</i>	Stream for more tokens

Returns

Success enumeration (1 if matched and assigned; -1 if matched, but there's some sort of error (i.e., too few args); 0 if not matched)

Definition at line 252 of file [pbsamparm.c](#).

7.13.5.12 PBSAMparm_parseTolsp()

```

VPRIVATE Vrc_Codes PBSAMparm_parseTolsp (
    PBSAMparm * thee,
    Vio * sock )

```

Find sphere tolerance for coarse-graining.

Author

Parameters

<i>thee</i>	PBSAMparm object to be copied into
<i>sock</i>	The stream from which parameter is taken

Definition at line 232 of file [pbsamparm.c](#).

7.14 Vacc class

Solvent- and ion-accessibility oracle.

Files

- file [vacc.c](#)
Class Vacc methods.
- file [vacc.h](#)
Contains declarations for class Vacc.

Data Structures

- struct [sVaccSurf](#)
Surface object list of per-atom surface points.
- struct [sVacc](#)
Oracle for solvent- and ion-accessibility around a biomolecule.

Typedefs

- typedef struct [sVaccSurf](#) [VaccSurf](#)
Declaration of the VaccSurf class as the VaccSurf structure.
- typedef struct [sVacc](#) [Vacc](#)
Declaration of the Vacc class as the Vacc structure.

Functions

- VEXTERNC unsigned long int [Vacc_memChk](#) ([Vacc](#) *thee)
Get number of bytes in this object and its members.
- VEXTERNC [VaccSurf](#) * [VaccSurf_ctor](#) (Vmem *mem, double probe_radius, int nsphere)
Allocate and construct the surface object; do not assign surface points to positions.
- VEXTERNC int [VaccSurf_ctor2](#) ([VaccSurf](#) *thee, Vmem *mem, double probe_radius, int nsphere)
Construct the surface object using previously allocated memory; do not assign surface points to positions.
- VEXTERNC void [VaccSurf_dtor](#) ([VaccSurf](#) **thee)
Destroy the surface object and free its memory.
- VEXTERNC void [VaccSurf_dtor2](#) ([VaccSurf](#) *thee)
Destroy the surface object.
- VEXTERNC [VaccSurf](#) * [VaccSurf_refSphere](#) (Vmem *mem, int npts)
Set up an array of points for a reference sphere of unit radius.
- VEXTERNC [VaccSurf](#) * [Vacc_atomSurf](#) ([Vacc](#) *thee, [Vatom](#) *atom, [VaccSurf](#) *ref, double probe_radius)
Set up an array of points corresponding to the SAS due to a particular atom.
- VEXTERNC [Vacc](#) * [Vacc_ctor](#) ([Valist](#) *alist, [Vclist](#) *clist, double surf_density)
Construct the accessibility object.
- VEXTERNC int [Vacc_ctor2](#) ([Vacc](#) *thee, [Valist](#) *alist, [Vclist](#) *clist, double surf_density)
FORTTRAN stub to construct the accessibility object.
- VEXTERNC void [Vacc_dtor](#) ([Vacc](#) **thee)
Destroy object.
- VEXTERNC void [Vacc_dtor2](#) ([Vacc](#) *thee)
FORTTRAN stub to destroy object.
- VEXTERNC double [Vacc_vdwAcc](#) ([Vacc](#) *thee, double center[[VAPBS_DIM](#)])

- Report van der Waals accessibility.*

 - VEXTERNC double `Vacc_ivdwAcc` (`Vacc` *three, double center[VAPBS_DIM], double radius)
- Report inflated van der Waals accessibility.*

 - VEXTERNC double `Vacc_molAcc` (`Vacc` *three, double center[VAPBS_DIM], double radius)
- Report molecular accessibility.*

 - VEXTERNC double `Vacc_fastMolAcc` (`Vacc` *three, double center[VAPBS_DIM], double radius)
- Report molecular accessibility quickly.*

 - VEXTERNC double `Vacc_splineAcc` (`Vacc` *three, double center[VAPBS_DIM], double win, double infrad)
- Report spline-based accessibility.*

 - VEXTERNC void `Vacc_splineAccGrad` (`Vacc` *three, double center[VAPBS_DIM], double win, double infrad, double *grad)
- Report gradient of spline-based accessibility.*

 - VEXTERNC double `Vacc_splineAccAtom` (`Vacc` *three, double center[VAPBS_DIM], double win, double infrad, `Vatom` *atom)
- Report spline-based accessibility for a given atom.*

 - VEXTERNC void `Vacc_splineAccGradAtomUnnorm` (`Vacc` *three, double center[VAPBS_DIM], double win, double infrad, `Vatom` *atom, double *force)
- Report gradient of spline-based accessibility with respect to a particular atom (see Vpmsg_splineAccAtom)*

 - VEXTERNC void `Vacc_splineAccGradAtomNorm` (`Vacc` *three, double center[VAPBS_DIM], double win, double infrad, `Vatom` *atom, double *force)
- Report gradient of spline-based accessibility with respect to a particular atom normalized by the accessibility value due to that atom at that point (see Vpmsg_splineAccAtom)*

 - VEXTERNC void `Vacc_splineAccGradAtomNorm4` (`Vacc` *three, double center[VAPBS_DIM], double win, double infrad, `Vatom` *atom, double *force)
- Report gradient of spline-based accessibility with respect to a particular atom normalized by a 4th order accessibility value due to that atom at that point (see Vpmsg_splineAccAtom)*

 - VEXTERNC void `Vacc_splineAccGradAtomNorm3` (`Vacc` *three, double center[VAPBS_DIM], double win, double infrad, `Vatom` *atom, double *force)
- Report gradient of spline-based accessibility with respect to a particular atom normalized by a 3rd order accessibility value due to that atom at that point (see Vpmsg_splineAccAtom)*

 - VEXTERNC double `Vacc_SASA` (`Vacc` *three, double radius)
- Build the solvent accessible surface (SAS) and calculate the solvent accessible surface area.*

 - VEXTERNC double `Vacc_totalSASA` (`Vacc` *three, double radius)
- Return the total solvent accessible surface area (SASA)*

 - VEXTERNC double `Vacc_atomSASA` (`Vacc` *three, double radius, `Vatom` *atom)
- Return the atomic solvent accessible surface area (SASA)*

 - VEXTERNC `VaccSurf` * `Vacc_atomSASPoints` (`Vacc` *three, double radius, `Vatom` *atom)
- Get the set of points for this atom's solvent-accessible surface.*

 - VEXTERNC void `Vacc_atomdSAV` (`Vacc` *three, double radius, `Vatom` *atom, double *dSA)
- Get the derivate of solvent accessible volume.*

 - VEXTERNC void `Vacc_atomdSASA` (`Vacc` *three, double dpos, double radius, `Vatom` *atom, double *dSA)
- Get the derivate of solvent accessible area.*

 - VEXTERNC void `Vacc_totalAtomdSASA` (`Vacc` *three, double dpos, double radius, `Vatom` *atom, double *dSA)
- Testing purposes only.*

 - VEXTERNC void `Vacc_totalAtomdSAV` (`Vacc` *three, double dpos, double radius, `Vatom` *atom, double *dSA, `Vclist` *clist)
- Total solvent accessible volume.*

 - VEXTERNC double `Vacc_totalSAV` (`Vacc` *three, `Vclist` *clist, `APOLparm` *apolparm, double radius)
- Return the total solvent accessible volume (SAV)*

- VEXTERNC int [Vacc_wcaEnergy](#) ([Vacc](#) *thee, [APOLparm](#) *apolparm, [Valist](#) *alist, [Vclist](#) *clist)
Return the WCA integral energy.
- VEXTERNC int [Vacc_wcaForceAtom](#) ([Vacc](#) *thee, [APOLparm](#) *apolparm, [Vclist](#) *clist, [Vatom](#) *atom, double *force)
Return the WCA integral force.
- VEXTERNC int [Vacc_wcaEnergyAtom](#) ([Vacc](#) *thee, [APOLparm](#) *apolparm, [Valist](#) *alist, [Vclist](#) *clist, int iatom, double *value)
Calculate the WCA energy for an atom.

7.14.1 Detailed Description

Solvent- and ion-accessibility oracle.

7.14.2 Typedef Documentation

7.14.2.1 Vacc

```
typedef struct sVacc Vacc
```

Declaration of the Vacc class as the Vacc structure.

Definition at line 131 of file [vacc.h](#).

7.14.2.2 VaccSurf

```
typedef struct sVaccSurf VaccSurf
```

Declaration of the VaccSurf class as the VaccSurf structure.

Definition at line 101 of file [vacc.h](#).

7.14.3 Function Documentation

7.14.3.1 Vacc_atomdSASA()

```
VEXTERNC void Vacc_atomdSASA (
    Vacc * thee,
    double dpos,
    double radius,
    Vatom * atom,
    double * dSA )
```

Get the derivative of solvent accessible area.

Author

Jason Wagoner, David Gohara, Nathan Baker

Parameters

<i>thee</i>	Accessability object
<i>dpos</i>	Atom position offset
<i>radius</i>	Probe radius (Å)
<i>atom</i>	Atom of interest
<i>dSA</i>	Array holding answers of calc

Definition at line 1320 of file [vacc.c](#).

7.14.3.2 Vacc_atomdSAV()

```
VEXTERNC void Vacc_atomdSAV (
    Vacc * thee,
    double radius,
    Vatom * atom,
    double * dSA )
```

Get the derivative of solvent accessible volume.

Author

Jason Wagoner, Nathan Baker

Parameters

<i>thee</i>	Accessibility object
<i>radius</i>	Probe radius (Å)
<i>atom</i>	Atom of interest
<i>dSA</i>	Array holding answers of calc

Definition at line 1200 of file [vacc.c](#).

7.14.3.3 Vacc_atomSASA()

```
VEXTERNC double Vacc_atomSASA (
    Vacc * thee,
    double radius,
    Vatom * atom )
```

Return the atomic solvent accessible surface area (SASA)

Note

Alias for Vacc_SASA

Author

Nathan Baker

Returns

Atomic solvent accessible area (Å²)

Parameters

<i>thee</i>	Accessibility object
<i>radius</i>	Probe molecule radius (Å)
<i>atom</i>	Atom of interest

Definition at line 780 of file [vacc.c](#).

7.14.3.4 Vacc_atomSASPoints()

```
VEXTERNC VaccSurf * Vacc_atomSASPoints (
    Vacc * thee,
```

```
double radius,  
Vatom * atom )
```

Get the set of points for this atom's solvent-accessible surface.

Author

Nathan Baker

Returns

Pointer to VaccSurf object for this atom

Parameters

<i>thee</i>	Accessibility object
<i>radius</i>	Probe molecule radius (Å)
<i>atom</i>	Atom of interest

Definition at line 982 of file [vacc.c](#).

7.14.3.5 Vacc_atomSurf()

```
VEXTERNC VaccSurf * Vacc_atomSurf (  
    Vacc * thee,  
    Vatom * atom,  
    VaccSurf * ref,  
    double probe_radius )
```

Set up an array of points corresponding to the SAS due to a particular atom.

Author

Nathan Baker

Returns

Atom sphere surface object

Parameters

<i>thee</i>	Accessibility object for molecule
<i>atom</i>	Atom for which the surface should be constructed
<i>ref</i>	Reference sphere which sets the resolution for the surface.

See also

[VaccSurf_refSphere](#)

Parameters

<i>probe_radius</i>	Probe radius (in Å)
---------------------	---------------------

Definition at line 868 of file [vacc.c](#).

7.14.3.6 Vacc_ctor()

```
VECTERNC Vacc * Vacc_ctor (
    Valist * alist,
    Vclist * clist,
    double surf_density )
```

Construct the accessibility object.

Author

Nathan Baker

Returns

Newly allocated Vacc object

Parameters

<i>alist</i>	Molecule for accessibility queries
<i>clist</i>	Pre-constructed cell list for looking up atoms near specific positions
<i>surf_density</i>	Minimum per-atom solvent accessible surface point density (in pts/A ²)

Definition at line 132 of file [vacc.c](#).

7.14.3.7 Vacc_ctor2()

```
VECTERNC int Vacc_ctor2 (
    Vacc * thee,
    Valist * alist,
    Vclist * clist,
    double surf_density )
```

FORTTRAN stub to construct the accessibility object.

Author

Nathan Baker

Returns

1 if successful, 0 otherwise

Parameters

<i>thee</i>	Memory for Vacc objet
<i>alist</i>	Molecule for accessibility queries
<i>clist</i>	Pre-constructed cell list for looking up atoms near specific positions
<i>surf_density</i>	Minimum per-atom solvent accessible surface point density (in pts/A ²)

Definition at line 213 of file [vacc.c](#).

7.14.3.8 Vacc_dtor()

```
VECTERNC void Vacc_dtor (
    Vacc ** thee )
```

Destroy object.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to memory location of object
-------------	--------------------------------------

Definition at line 245 of file [vacc.c](#).

7.14.3.9 Vacc_dtor2()

```
VEXTERNC void Vacc_dtor2 (  
    Vacc * thee )
```

FORTTRAN stub to destroy object.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to object
-------------	-------------------

Definition at line 255 of file [vacc.c](#).

7.14.3.10 Vacc_fastMolAcc()

```
VEXTERNC double Vacc_fastMolAcc (  
    Vacc * thee,  
    double center[VAPBS_DIM],  
    double radius )
```

Report molecular accessibility quickly.

Given a point which is INSIDE the collection of inflated van der Waals spheres, but OUTSIDE the collection of non-inflated van der Waals spheres, determine accessibility of a probe (of radius radius) at a given point, given a collection of atomic spheres. Uses molecular (Connolly) surface definition.

Note

THIS ASSUMES YOU HAVE TESTED THAT THIS POINT IS DEFINITELY INSIDE THE INFLATED AND NON-
INFLATED VAN DER WAALS SURFACES!

Author

Nathan Baker

Returns

Characteristic function value between 1.0 (accessible) and 0.0 (inaccessible)

Bug This routine has a slight bug which can generate very small internal regions of high dielectric (thanks to John Mongan and Jess Swanson for finding this)

Parameters

<i>thee</i>	Accessibility object
<i>center</i>	Probe center coordinates
<i>radius</i>	Probe radius (in Å)

Definition at line 637 of file [vacc.c](#).

7.14.3.11 Vacc_ivdwAcc()

```
VEXTERNC double Vacc_ivdwAcc (  
    Vacc * thee,  
    double center[VAPBS_DIM],  
    double radius )
```

Report inflated van der Waals accessibility.

Determines if a point is within the union of the spheres centered at the atomic centers with radii equal to the sum of the atomic van der Waals radius and the probe radius.

Author

Nathan Baker

Returns

Characteristic function value between 1.0 (accessible) and 0.0 (inaccessible)

Parameters

<i>thee</i>	Accessibility object
<i>center</i>	Probe center coordinates
<i>radius</i>	Probe radius (Å)

7.14.3.12 Vacc_memChk()

```
VEXTERNC unsigned long int Vacc_memChk (  
    Vacc * thee )
```

Get number of bytes in this object and its members.

Author

Nathan Baker

Returns

Number of bytes allocated for object

Parameters

<i>thee</i>	Object for memory check
-------------	-------------------------

Definition at line 63 of file [vacc.c](#).

7.14.3.13 Vacc_molAcc()

```
VECTERNC double Vacc_molAcc (  
    Vacc * thee,  
    double center[VAPBS_DIM],  
    double radius )
```

Report molecular accessibility.

Determine accessibility of a probe (of radius radius) at a given point, given a collection of atomic spheres. Uses molecular (Connolly) surface definition.

Author

Nathan Baker

Returns

Characteristic function value between 1.0 (accessible) and 0.0 (inaccessible)

Bug This routine has a slight bug which can generate very small internal regions of high dielectric (thanks to John Mongan and Jess Swanson for finding this)

Parameters

<i>thee</i>	Accessibility object
<i>center</i>	Probe center coordinates
<i>radius</i>	Probe radius (in Å)

Definition at line 608 of file [vacc.c](#).

7.14.3.14 Vacc_SASA()

```
VECTERNC double Vacc_SASA (  
    Vacc * thee,  
    double radius )
```

Build the solvent accessible surface (SAS) and calculate the solvent accessible surface area.

Note

Similar to UHBD FORTRAN routine by Brock Luty (returns UHBD's asas2)

Author

Nathan Baker (original FORTRAN routine by Brock Luty)

Returns

Total solvent accessible area (Å²)

Parameters

<i>thee</i>	Accessibility object
<i>radius</i>	Probe molecule radius (Å)

Definition at line 713 of file [vacc.c](#).

7.14.3.15 Vacc_splineAcc()

```
VEXTERNC double Vacc_splineAcc (
    Vacc * thee,
    double center[VAPBS_DIM],
    double win,
    double infrad )
```

Report spline-based accessibility.

Determine accessibility at a given point, given a collection of atomic spheres. Uses Benoit Roux (Im et al, Comp Phys Comm, 111, 59–75, 1998) definition suitable for force evaluation; basically a cubic spline.

Author

Nathan Baker

Returns

Characteristic function value between 1.0 (accessible) and 0.0 (inaccessible)

Parameters

<i>thee</i>	Accessibility object
<i>center</i>	Probe center coordinates
<i>win</i>	Spline window (Å)
<i>infrad</i>	Inflation radius (Å) for ion access.

Definition at line 528 of file [vacc.c](#).

7.14.3.16 Vacc_splineAccAtom()

```
VEXTERNC double Vacc_splineAccAtom (
    Vacc * thee,
    double center[VAPBS_DIM],
    double win,
    double infrad,
    Vatom * atom )
```

Report spline-based accessibility for a given atom.

Determine accessibility at a given point for a given atomic spheres. Uses Benoit Roux (Im et al, Comp Phys Comm, 111, 59–75, 1998) definition suitable for force evaluation; basically a cubic spline.

Author

Nathan Baker

Returns

Characteristic function value between 1.0 (accessible) and 0.0 (inaccessible)

Parameters

<i>thee</i>	Accessibility object
<i>center</i>	Probe center coordinates
<i>win</i>	Spline window (Å)
<i>infrad</i>	Inflation radius (Å) for ion access.
<i>atom</i>	Atom

Definition at line 438 of file [vacc.c](#).

7.14.3.17 Vacc_splineAccGrad()

```
VEXTERNC void Vacc_splineAccGrad (
    Vacc * thee,
    double center[VAPBS_DIM],
    double win,
    double infrad,
    double * grad )
```

Report gradient of spline-based accessibility.

Author

Nathan Baker

Parameters

<i>thee</i>	Accessibility object
<i>center</i>	Probe center coordinates
<i>win</i>	Spline window (Å)
<i>infrad</i>	Inflation radius (Å) for ion access.
<i>grad</i>	3-vector set to gradient of accessibility

Definition at line 561 of file [vacc.c](#).

7.14.3.18 Vacc_splineAccGradAtomNorm()

```
VEXTERNC void Vacc_splineAccGradAtomNorm (
    Vacc * thee,
    double center[VAPBS_DIM],
    double win,
    double infrad,
    Vatom * atom,
    double * force )
```

Report gradient of spline-based accessibility with respect to a particular atom normalized by the accessibility value due to that atom at that point (see [Vpmg_splineAccAtom](#))

Determine accessibility at a given point, given a collection of atomic spheres. Uses Benoit Roux (Im et al, Comp Phys Comm, 111, 59–75, 1998) definition suitable for force evalation; basically a cubic spline.

Author

Nathan Baker

Parameters

<i>thee</i>	Accessibility object
<i>center</i>	Probe center coordinates
<i>win</i>	Spline window (Å)
<i>infrad</i>	Inflation radius (Å) for ion access.
<i>atom</i>	Atom
<i>force</i>	VAPBS_DIM-vector set to gradient of accessibility

Definition at line 316 of file [vacc.c](#).

7.14.3.19 Vacc_splineAccGradAtomNorm3()

```
VEXTERNC void Vacc_splineAccGradAtomNorm3 (
    Vacc * thee,
    double center[VAPBS_DIM],
    double win,
    double infrad,
    Vatom * atom,
    double * force )
```

Report gradient of spline-based accessibility with respect to a particular atom normalized by a 3rd order accessibility value due to that atom at that point (see [Vpmg_splineAccAtom](#))

Author

Michael Schnieders

Parameters

<i>thee</i>	Accessibility object
<i>center</i>	Probe center coordinates
<i>win</i>	Spline window (Å)
<i>infrad</i>	Inflation radius (Å) for ion access.
<i>atom</i>	Atom
<i>force</i>	VAPBS_DIM-vector set to gradient of accessibility

Definition at line 1099 of file [vacc.c](#).

7.14.3.20 Vacc_splineAccGradAtomNorm4()

```
VEXTERNC void Vacc_splineAccGradAtomNorm4 (
    Vacc * thee,
    double center[VAPBS_DIM],
    double win,
    double infrad,
    Vatom * atom,
    double * force )
```

Report gradient of spline-based accessibility with respect to a particular atom normalized by a 4th order accessibility value due to that atom at that point (see [Vpmg_splineAccAtom](#))

Author

Michael Schnieders

Parameters

<i>thee</i>	Accessibility object
<i>center</i>	Probe center coordinates
<i>win</i>	Spline window (Å)
<i>infrad</i>	Inflation radius (Å) for ion access.
<i>atom</i>	Atom
<i>force</i>	VAPBS_DIM-vector set to gradient of accessibility

Definition at line 1006 of file [vacc.c](#).

7.14.3.21 Vacc_splineAccGradAtomUnnorm()

```

VEXTERNC void Vacc_splineAccGradAtomUnnorm (
    Vacc * thee,
    double center[VAPBS_DIM],
    double win,
    double infrad,
    Vatom * atom,
    double * force )

```

Report gradient of spline-based accessibility with respect to a particular atom (see `Vpmg_splineAccAtom`)
Determine accessibility at a given point, given a collection of atomic spheres. Uses Benoit Roux (Im et al, Comp Phys Comm, 111, 59–75, 1998) definition suitable for force evalation; basically a cubic spline.

Author

Nathan Baker

Parameters

<i>thee</i>	Accessibility object
<i>center</i>	Probe center coordinates
<i>win</i>	Spline window (Å)
<i>infrad</i>	Inflation radius (Å) for ion access.
<i>atom</i>	Atom
<i>force</i>	VAPBS_DIM-vector set to gradient of accessibility

Definition at line 377 of file [vacc.c](#).

7.14.3.22 Vacc_totalAtomdSASA()

```

VEXTERNC void Vacc_totalAtomdSASA (
    Vacc * thee,
    double dpos,
    double radius,
    Vatom * atom,
    double * dSA )

```

Testing purposes only.

Author

David Gohara, Nathan Baker

Parameters

<i>thee</i>	Accessibility object
<i>dpos</i>	Atom position offset
<i>radius</i>	Probe radius (Å)
<i>atom</i>	Atom of interest
<i>dSA</i>	Array holding answers of calc

Definition at line 1389 of file [vacc.c](#).

7.14.3.23 Vacc_totalAtomdSAV()

```
VEXTERNC void Vacc_totalAtomdSAV (
    Vacc * thee,
    double dpos,
    double radius,
    Vatom * atom,
    double * dSA,
    Vclist * clist )
```

Total solvent accessible volume.

Author

David Gohara, Nathan Baker

Parameters

<i>thee</i>	Accessibility object
<i>dpos</i>	Atom position offset
<i>radius</i>	Probe radius (Å)
<i>atom</i>	Atom of interest
<i>dSA</i>	Array holding answers of calc
<i>clist</i>	clist for this calculation

Definition at line 1448 of file [vacc.c](#).

7.14.3.24 Vacc_totalSASA()

```
VEXTERNC double Vacc_totalSASA (
    Vacc * thee,
    double radius )
```

Return the total solvent accessible surface area (SASA)

Note

Alias for Vacc_SASA

Author

Nathan Baker

Returns

Total solvent accessible area (Å²)

Parameters

<i>thee</i>	Accessibility object
<i>radius</i>	Probe molecule radius (Å)

Definition at line 774 of file [vacc.c](#).

7.14.3.25 Vacc_totalSAV()

```
VEXTERNC double Vacc_totalSAV (  
    Vacc * thee,  
    Vclist * clist,  
    APOLparm * apolparm,  
    double radius )
```

Return the total solvent accessible volume (SAV)

Note

Alias for Vacc_SAV

Author

David Gohara

Returns

Total solvent accessible volume (\AA^3)

Parameters

<i>thee</i>	Accessibility object
<i>clist</i>	Clist for acc object
<i>apolparm</i>	Apolar parameters – could be VNULL if none required for this calculation. If VNULL, then default settings are used
<i>radius</i>	Probe molecule radius (\AA)

Definition at line 1503 of file [vacc.c](#).

7.14.3.26 Vacc_vdwAcc()

```
VEXTERNC double Vacc_vdwAcc (  
    Vacc * thee,  
    double center[VAPBS_DIM] )
```

Report van der Waals accessibility.

Determines if a point is within the union of the atomic spheres (with radii equal to their van der Waals radii).

Author

Nathan Baker

Returns

Characteristic function value between 1.0 (accessible) and 0.0 (inaccessible)

Parameters

<i>thee</i>	Accessibility object
<i>center</i>	Probe center coordinates

7.14.3.27 Vacc_wcaEnergy()

```
VEXTERNC int Vacc_wcaEnergy (
    Vacc * thee,
    APOLparm * apolparm,
    Valist * alist,
    Vclist * clist )
```

Return the WCA integral energy.

Author

David Gohara

Returns

Success flag

Parameters

<i>thee</i>	Accessibility object
<i>apolparm</i>	Apolar calculation parameters
<i>alist</i>	Alist for acc object
<i>clist</i>	Clist for acc object

Definition at line 1721 of file [vacc.c](#).

7.14.3.28 Vacc_wcaEnergyAtom()

```
VEXTERNC int Vacc_wcaEnergyAtom (
    Vacc * thee,
    APOLparm * apolparm,
    Valist * alist,
    Vclist * clist,
    int iatom,
    double * value )
```

Calculate the WCA energy for an atom.

Author

Dave Gohara and Nathan Baker

Returns

Success flag

Parameters

<i>thee</i>	Accessibility object
<i>apolparm</i>	Apolar calculation parameters
<i>alist</i>	Atom list
<i>clist</i>	Cell list associated with Vacc object
<i>iatom</i>	Index for atom of interest
<i>value</i>	Set to energy value

Definition at line 1580 of file [vacc.c](#).

7.14.3.29 Vacc_wcaForceAtom()

```
VEXTERNC int Vacc_wcaForceAtom (
    Vacc * thee,
    APOLparm * apolparm,
    Vclist * clist,
    Vatom * atom,
    double * force )
```

Return the WCA integral force.

Author

David Gohara

Returns

WCA energy (kJ/mol/A)

Parameters

<i>thee</i>	Accessibility object
<i>apolparm</i>	Apolar calculation parameters
<i>clist</i>	Clist for acc object
<i>atom</i>	Current atom
<i>force</i>	Force for atom

Definition at line 1756 of file [vacc.c](#).

7.14.3.30 VaccSurf_ctor()

```
VEXTERNC VaccSurf * VaccSurf_ctor (
    Vmem * mem,
    double probe_radius,
    int nsphere )
```

Allocate and construct the surface object; do not assign surface points to positions.

Author

Nathan Baker

Returns

Newly allocated and constructed surface object

Parameters

<i>mem</i>	Memory manager (can be VNULL)
<i>probe_radius</i>	Probe radius (in A) for this surface
<i>nsphere</i>	Number of points in sphere

Definition at line 803 of file [vacc.c](#).

7.14.3.31 VaccSurf_ctor2()

```

VEXTERNC int VaccSurf_ctor2 (
    VaccSurf * thee,
    Vmem * mem,
    double probe_radius,
    int nsphere )

```

Construct the surface object using previously allocated memory; do not assign surface points to positions.

Author

Nathan Baker

Returns

1 if successful, 0 otherwise

Parameters

<i>thee</i>	Allocated memory
<i>mem</i>	Memory manager (can be VNULL)
<i>probe_radius</i>	Probe radius (in A) for this surface
<i>nsphere</i>	Number of points in sphere

Definition at line 813 of file [vacc.c](#).

7.14.3.32 VaccSurf_dtor()

```

VEXTERNC void VaccSurf_dtor (
    VaccSurf ** thee )

```

Destroy the surface object and free its memory.

Author

Nathan Baker

Parameters

<i>thee</i>	Object to be destroyed
-------------	------------------------

Definition at line 839 of file [vacc.c](#).

7.14.3.33 VaccSurf_dtor2()

```

VEXTERNC void VaccSurf_dtor2 (
    VaccSurf * thee )

```

Destroy the surface object.

Author

Nathan Baker

Parameters

<i>thee</i>	Object to be destroyed
-------------	------------------------

Definition at line 853 of file [vacc.c](#).

7.14.3.34 VaccSurf_refSphere()

```

VEXTERNC VaccSurf * VaccSurf_refSphere (
    Vmem * mem,
    int npts )

```

Set up an array of points for a reference sphere of unit radius.

Generates approximately npts # of points (actual number stored in thee->npts) somewhat uniformly distributed across a sphere of unit radius centered at the origin.

Note

This routine was shamelessly ripped off from sphere.f from UHBD as developed by Michael K. Gilson.

Author

Nathan Baker (original FORTRAN code by Mike Gilson)

Returns

Reference sphere surface object

Parameters

<i>mem</i>	Memory object
<i>npts</i>	Requested number of points on sphere

Definition at line 926 of file [vacc.c](#).

7.15 Valist class

Container class for list of atom objects.

Files

- file [valist.h](#)
Contains declarations for class Valist.

Data Structures

- struct [sValist](#)
Container class for list of atom objects.

Typedefs

- typedef struct [sValist](#) Valist
Declaration of the Valist class as the Valist structure.

Functions

- VEXTERNC [Vatom](#) * [Valist_getAtomList](#) ([Valist](#) *thee)
Get actual array of atom objects from the list.

- VEXTERNC double [Valist_getCenterX](#) ([Valist](#) *thee)
Get x-coordinate of molecule center.
- VEXTERNC double [Valist_getCenterY](#) ([Valist](#) *thee)
Get y-coordinate of molecule center.
- VEXTERNC double [Valist_getCenterZ](#) ([Valist](#) *thee)
Get z-coordinate of molecule center.
- VEXTERNC int [Valist_getNumberAtoms](#) ([Valist](#) *thee)
Get number of atoms in the list.
- VEXTERNC [Vatom](#) * [Valist_getAtom](#) ([Valist](#) *thee, int i)
Get pointer to particular atom in list.
- VEXTERNC unsigned long int [Valist_memChk](#) ([Valist](#) *thee)
Get total memory allocated for this object and its members.
- VEXTERNC [Valist](#) * [Valist_ctor](#) ()
Construct the atom list object.
- VEXTERNC [Vrc_Codes](#) [Valist_ctor2](#) ([Valist](#) *thee)
FORTTRAN stub to construct the atom list object.
- VEXTERNC void [Valist_dtor](#) ([Valist](#) **thee)
Destroys atom list object.
- VEXTERNC void [Valist_dtor2](#) ([Valist](#) *thee)
FORTTRAN stub to destroy atom list object.
- VEXTERNC [Vrc_Codes](#) [Valist_readPQR](#) ([Valist](#) *thee, [Vparam](#) *param, [Vio](#) *sock)
Fill atom list with information from a PQR file.
- VEXTERNC [Vrc_Codes](#) [Valist_readPDB](#) ([Valist](#) *thee, [Vparam](#) *param, [Vio](#) *sock)
Fill atom list with information from a PDB file.
- VEXTERNC [Vrc_Codes](#) [Valist_readXML](#) ([Valist](#) *thee, [Vparam](#) *param, [Vio](#) *sock)
Fill atom list with information from an XML file.
- VEXTERNC [Vrc_Codes](#) [Valist_getStatistics](#) ([Valist](#) *thee)
Load up Valist with various statistics.

7.15.1 Detailed Description

Container class for list of atom objects.

7.15.2 Typedef Documentation

7.15.2.1 Valist

```
typedef struct sValist Valist
```

Declaration of the Valist class as the Valist structure.

Definition at line 95 of file [valist.h](#).

7.15.3 Function Documentation

7.15.3.1 Valist_ctor()

```
VEXTERNC Valist * Valist_ctor ( )
```

Construct the atom list object.

Author

Nathan Baker

Returns

Pointer to newly allocated (empty) atom list

Definition at line 138 of file [valist.c](#).

7.15.3.2 Valist_ctor2()

```
VEXTERNC Vrc_Codes Valist_ctor2 (  
    Valist * thee )
```

FORTTRAN stub to construct the atom list object.

Author

Nathan Baker, Yong Huang

Returns

Success enumeration

Parameters

<i>thee</i>	Storage for new atom list
-------------	---------------------------

Definition at line 155 of file [valist.c](#).

7.15.3.3 Valist_dtor()

```
VEXTERNC void Valist_dtor (  
    Valist ** thee )
```

Destroys atom list object.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to storage for atom list
-------------	----------------------------------

Definition at line 167 of file [valist.c](#).

7.15.3.4 Valist_dtor2()

```
VEXTERNC void Valist_dtor2 (  
    Valist * thee )
```

FORTTRAN stub to destroy atom list object.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to atom list object
-------------	-----------------------------

Definition at line 176 of file [valist.c](#).

7.15.3.5 Valist_getAtom()

```
VEXTERNC Vatom * Valist_getAtom (
    Valist * thee,
    int i )
```

Get pointer to particular atom in list.

Author

Nathan Baker

Returns

Pointer to atom object i

Parameters

<i>thee</i>	Atom list object
<i>i</i>	Index of atom in list

Definition at line 115 of file [valist.c](#).

7.15.3.6 Valist_getAtomList()

```
VEXTERNC Vatom * Valist_getAtomList (
    Valist * thee )
```

Get actual array of atom objects from the list.

Author

Nathan Baker

Returns

Array of atom objects

Parameters

<i>thee</i>	Atom list object
-------------	------------------

Definition at line 95 of file [valist.c](#).

7.15.3.7 Valist_getCenterX()

```
VEXTERNC double Valist_getCenterX (
    Valist * thee )
```

Get x-coordinate of molecule center.

Author

Nathan Baker

Returns

X-coordinate of molecule center

Parameters

<i>thee</i>	Atom list object
-------------	------------------

Definition at line 66 of file [valist.c](#).

7.15.3.8 Valist_getCenterY()

```
VEXTERNC double Valist_getCenterY (  
    Valist * thee )
```

Get y-coordinate of molecule center.

Author

Nathan Baker

Returns

Y-coordinate of molecule center

Parameters

<i>thee</i>	Atom list object
-------------	------------------

Definition at line 76 of file [valist.c](#).

7.15.3.9 Valist_getCenterZ()

```
VEXTERNC double Valist_getCenterZ (  
    Valist * thee )
```

Get z-coordinate of molecule center.

Author

Nathan Baker

Returns

Z-coordinate of molecule center

Parameters

<i>thee</i>	Atom list object
-------------	------------------

Definition at line 85 of file [valist.c](#).

7.15.3.10 Valist_getNumberAtoms()

```
VEXTERNC int Valist_getNumberAtoms (  
    Valist * thee )
```

Get number of atoms in the list.

Author

Nathan Baker

Returns

Number of atoms in list

Parameters

<i>thee</i>	Atom list object
-------------	------------------

Definition at line 105 of file [valist.c](#).

7.15.3.11 Valist_getStatistics()

```
VEXTERNC Vrc_Codes Valist_getStatistics (  
    Valist * thee )
```

Load up Valist with various statistics.

Author

Nathan Baker, Yong Huang

Returns

Success enumeration

Definition at line 869 of file [valist.c](#).

7.15.3.12 Valist_memChk()

```
VEXTERNC unsigned long int Valist_memChk (  
    Valist * thee )
```

Get total memory allocated for this object and its members.

Author

Nathan Baker

Returns

Total memory in bytes

Parameters

<i>thee</i>	Atom list object
-------------	------------------

Definition at line 129 of file [valist.c](#).

7.15.3.13 Valist_readPDB()

```
VEXTERNC Vrc_Codes Valist_readPDB (  
    Valist * thee,  
    Vparam * param,  
    Vio * sock )
```

Fill atom list with information from a PDB file.

Author

Nathan Baker, Todd Dolinsky, Yong Huang

Returns

Success enumeration

Note

We don't actually respect PDB format; instead recognize whitespace- or tab-delimited fields which allows us to deal with structures with coordinates > 999 or < -999 .

Parameters

<i>thee</i>	Atom list object
<i>param</i>	A pre-initialized parameter object
<i>sock</i>	Socket read for reading PDB file

Definition at line 515 of file [valist.c](#).

7.15.3.14 Valist_readPQR()

```
VEXTERNC Vrc_Codes Valist_readPQR (  
    Valist * thee,  
    Vparam * param,  
    Vio * sock )
```

Fill atom list with information from a PQR file.

Author

Nathan Baker, Yong Huang

Returns

Success enumeration

Note

- A PQR file has PDB structure with charge and radius in the last two columns instead of weight and occupancy
- We don't actually respect PDB format; instead recognize whitespace- or tab-delimited fields which allows us to deal with structures with coordinates > 999 or < -999 .

Parameters

<i>thee</i>	Atom list object
<i>param</i>	A pre-initialized parameter object
<i>sock</i>	Socket reading for reading PQR file

Definition at line 606 of file [valist.c](#).

7.15.3.15 Valist_readXML()

```

VEXTERNC Vrc_Codes Valist_readXML (
    Valist * thee,
    Vparam * param,
    Vio * sock )

```

Fill atom list with information from an XML file.

Author

Todd Dolinsky, Yong Huang

Returns

Success enumeration

Note

- The XML file must adhere to some guidelines, notably the presence of an <atom> tag with all other useful information (x, y, z, charge, and radius) as nested elements.

Parameters

<i>thee</i>	Atom list object
<i>param</i>	A pre-initialized parameter object
<i>sock</i>	Socket reading for reading PQR file

Definition at line 725 of file [valist.c](#).

7.16 Vatom class

Atom class for interfacing APBS with PDB files.

Files

- file [vatom.c](#)
Class Vatom methods.
- file [vatom.h](#)
Contains declarations for class Vatom.

Data Structures

- struct [sVatom](#)
Contains public data members for Vatom class/module.

Macros

- #define [VMAX_RECLEN](#) 64
Residue name length.

Typedefs

- typedef struct [sVatom](#) [Vatom](#)
Declaration of the Vatom class as the Vatom structure.

Functions

- VEXTERNC double * [Vatom_getPosition](#) ([Vatom](#) *thee)
Get atomic position.
- VEXTERNC void [Vatom_setRadius](#) ([Vatom](#) *thee, double radius)
Set atomic radius.
- VEXTERNC double [Vatom_getRadius](#) ([Vatom](#) *thee)
Get atomic position.
- VEXTERNC void [Vatom_setPartID](#) ([Vatom](#) *thee, int partID)
Set partition ID.
- VEXTERNC double [Vatom_getPartID](#) ([Vatom](#) *thee)
Get partition ID.
- VEXTERNC void [Vatom_setAtomID](#) ([Vatom](#) *thee, int id)
Set atom ID.
- VEXTERNC double [Vatom_getAtomID](#) ([Vatom](#) *thee)
Get atom ID.
- VEXTERNC void [Vatom_setCharge](#) ([Vatom](#) *thee, double charge)
Set atomic charge.
- VEXTERNC double [Vatom_getCharge](#) ([Vatom](#) *thee)
Get atomic charge.
- VEXTERNC void [Vatom_setEpsilon](#) ([Vatom](#) *thee, double epsilon)
Set atomic epsilon.
- VEXTERNC double [Vatom_getEpsilon](#) ([Vatom](#) *thee)
Get atomic epsilon.
- VEXTERNC unsigned long int [Vatom_memChk](#) ([Vatom](#) *thee)
Return the memory used by this structure (and its contents) in bytes.
- VEXTERNC void [Vatom_setResName](#) ([Vatom](#) *thee, char resName[VMAX_RECLEN])
Set residue name.
- VEXTERNC void [Vatom_setAtomName](#) ([Vatom](#) *thee, char atomName[VMAX_RECLEN])
Set atom name.
- VEXTERNC void [Vatom_getResName](#) ([Vatom](#) *thee, char resName[VMAX_RECLEN])
Retrieve residue name.
- VEXTERNC void [Vatom_getAtomName](#) ([Vatom](#) *thee, char atomName[VMAX_RECLEN])
Retrieve atom name.
- VEXTERNC [Vatom](#) * [Vatom_ctor](#) ()
Constructor for the Vatom class.
- VEXTERNC int [Vatom_ctor2](#) ([Vatom](#) *thee)
FORTTRAN stub constructor for the Vatom class.
- VEXTERNC void [Vatom_dtor](#) ([Vatom](#) **thee)
Object destructor.
- VEXTERNC void [Vatom_dtor2](#) ([Vatom](#) *thee)
FORTTRAN stub object destructor.
- VEXTERNC void [Vatom_setPosition](#) ([Vatom](#) *thee, double position[3])
Set the atomic position.
- VEXTERNC void [Vatom_copyTo](#) ([Vatom](#) *thee, [Vatom](#) *dest)
Copy information to another atom.
- VEXTERNC void [Vatom_copyFrom](#) ([Vatom](#) *thee, [Vatom](#) *src)
Copy information to another atom.

7.16.1 Detailed Description

Atom class for interfacing APBS with PDB files.

7.16.2 Macro Definition Documentation

7.16.2.1 VMAX_RECLEN

```
#define VMAX_RECLEN 64
```

Residue name length.

Author

Nathan Baker, David Gohara, Mike Schneiders

Definition at line 77 of file [vatom.h](#).

7.16.3 Typedef Documentation

7.16.3.1 Vatom

```
typedef struct sVatom Vatom
```

Declaration of the Vatom class as the Vatom structure.

Definition at line 114 of file [vatom.h](#).

7.16.4 Function Documentation

7.16.4.1 Vatom_copyFrom()

```
VEXTERNC void Vatom_copyFrom (
    Vatom * thee,
    Vatom * src )
```

Copy information to another atom.

Author

Nathan Baker

Parameters

<i>thee</i>	Destination for atom information
<i>src</i>	Source for atom information

Definition at line 186 of file [vatom.c](#).

7.16.4.2 Vatom_copyTo()

```
VEXTERNC void Vatom_copyTo (
    Vatom * thee,
    Vatom * dest )
```

Copy information to another atom.

Author

Nathan Baker

Parameters

<i>thee</i>	Source for atom information
<i>dest</i>	Destination for atom information

Definition at line 177 of file [vatom.c](#).

7.16.4.3 Vatom_ctor()

```
VEXTERNC Vatom * Vatom_ctor ( )
```

Constructor for the Vatom class.

Author

Nathan Baker

Returns

Pointer to newly allocated Vatom object

Definition at line 142 of file [vatom.c](#).

7.16.4.4 Vatom_ctor2()

```
VEXTERNC int Vatom_ctor2 (
    Vatom * thee )
```

FORTTRAN stub constructor for the Vatom class.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to Vatom allocated memory location
-------------	--

Returns

1 if succesful, 0 otherwise

Definition at line 153 of file [vatom.c](#).

7.16.4.5 Vatom_dtor()

```
VEXTERNC void Vatom_dtor (
    Vatom ** thee )
```

Object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to memory location of object to be destroyed
-------------	--

Definition at line 158 of file [vatom.c](#).

7.16.4.6 Vatom_dtor2()

```
VEXTERNC void Vatom_dtor2 (  
    Vatom * thee )
```

FORTTRAN stub object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to object to be destroyed
-------------	-----------------------------------

Definition at line 166 of file [vatom.c](#).

7.16.4.7 Vatom_getAtomID()

```
VEXTERNC double Vatom_getAtomID (  
    Vatom * thee )
```

Get atom ID.

Author

Nathan Baker

Parameters

<i>thee</i>	Vatom object
-------------	--------------

Returns

Unique non-negative number

Definition at line 84 of file [vatom.c](#).

7.16.4.8 Vatom_getAtomName()

```
VEXTERNC void Vatom_getAtomName (  
    Vatom * thee,  
    char atomName[VMAX_RECLEN] )
```

Retrieve atom name.

Author

Jason Wagoner

Parameters

<i>thee</i>	Vatom object
<i>atomName</i>	Atom name

Definition at line 214 of file [vatom.c](#).

7.16.4.9 Vatom_getCharge()

```
VEXTERNC double Vatom_getCharge (  
    Vatom * thee )
```

Get atomic charge.

Author

Nathan Baker

Parameters

<i>thee</i>	Vatom object
-------------	--------------

Returns

Atom partial charge (in e)

Definition at line 119 of file [vatom.c](#).

7.16.4.10 Vatom_getEpsilon()

```
VEXTERNC double Vatom_getEpsilon (  
    Vatom * thee )
```

Get atomic epsilon.

Author

David Gohara

Parameters

<i>thee</i>	Vatom object
-------------	--------------

Returns

Atomic epsilon (in Å)

Definition at line 132 of file [vatom.c](#).

7.16.4.11 Vatom_getPartID()

```
VEXTERNC double Vatom_getPartID (  
    Vatom * thee )
```

Get partition ID.

Author

Nathan Baker

Parameters

<i>thee</i>	Vatom object
-------------	--------------

Returns

Partition ID; a negative value means this atom is not assigned to any partition

Definition at line 70 of file [vatom.c](#).

7.16.4.12 Vatom_getPosition()

```
VEXTERNC double * Vatom_getPosition (
    Vatom * thee )
```

Get atomic position.

Author

Nathan Baker

Parameters

<i>thee</i>	Vatom object
-------------	--------------

Returns

Pointer to 3*double array of atomic coordinates (in Å)

Definition at line 63 of file [vatom.c](#).

7.16.4.13 Vatom_getRadius()

```
VEXTERNC double Vatom_getRadius (
    Vatom * thee )
```

Get atomic position.

Author

Nathan Baker

Parameters

<i>thee</i>	Vatom object
-------------	--------------

Returns

Atomic radius (in Å)

Definition at line 105 of file [vatom.c](#).

7.16.4.14 Vatom_getResName()

```
VEXTERNC void Vatom_getResName (
    Vatom * thee,
    char resName[VMAX_RECLEN] )
```

Retrieve residue name.

Author

Jason Wagoner

Parameters

<i>thee</i>	Vatom object
<i>resName</i>	Residue Name

Definition at line 199 of file [vatom.c](#).

7.16.4.15 Vatom_memChk()

```
VEXTERNC unsigned long int Vatom_memChk (  
    Vatom * thee )
```

Return the memory used by this structure (and its contents) in bytes.

Author

Nathan Baker

Parameters

<i>thee</i>	Vpmg object
-------------	-------------

Returns

The memory used by this structure and its contents in bytes

Definition at line 138 of file [vatom.c](#).

7.16.4.16 Vatom_setAtomID()

```
VEXTERNC void Vatom_setAtomID (  
    Vatom * thee,  
    int id )
```

Set atom ID.

Author

Nathan Baker

Parameters

<i>thee</i>	Vatom object
<i>id</i>	Unique non-negative number

Definition at line 91 of file [vatom.c](#).

7.16.4.17 Vatom_setAtomName()

```
VEXTERNC void Vatom_setAtomName (  
    Vatom * thee,  
    char atomName[VMAX_RECLEN] )
```

Set atom name.

Author

Jason Wagoner

Parameters

<i>thee</i>	Vatom object
<i>atomName</i>	Atom name

Definition at line 207 of file [vatom.c](#).**7.16.4.18 Vatom_setCharge()**

```
VEXTERNC void Vatom_setCharge (
    Vatom * thee,
    double charge )
```

Set atomic charge.

Author

Nathan Baker

Parameters

<i>thee</i>	Vatom object
<i>charge</i>	Atom partial charge (in e)

Definition at line 112 of file [vatom.c](#).**7.16.4.19 Vatom_setEpsilon()**

```
VEXTERNC void Vatom_setEpsilon (
    Vatom * thee,
    double epsilon )
```

Set atomic epsilon.

Author

David Gohara

Parameters

<i>thee</i>	Vatom object
<i>epsilon</i>	Atomic epsilon (in Å)

Definition at line 126 of file [vatom.c](#).**7.16.4.20 Vatom_setPartID()**

```
VEXTERNC void Vatom_setPartID (
    Vatom * thee,
    int partID )
```

Set partition ID.

Author

Nathan Baker

Parameters

<i>thee</i>	Vatom object
<i>partID</i>	Partition ID; a negative value means this atom is not assigned to any partition

Definition at line 77 of file [vatom.c](#).

7.16.4.21 Vatom_setPosition()

```
VEXTERNC void Vatom_setPosition (
    Vatom * thee,
    double position[3] )
```

Set the atomic position.

Author

Nathan Baker

Parameters

<i>thee</i>	Vatom object to be modified
<i>position</i>	Coordinates (in Å)

Definition at line 168 of file [vatom.c](#).

7.16.4.22 Vatom_setRadius()

```
VEXTERNC void Vatom_setRadius (
    Vatom * thee,
    double radius )
```

Set atomic radius.

Author

Nathan Baker

Parameters

<i>thee</i>	Vatom object
<i>radius</i>	Atomic radius (in Å)

Definition at line 98 of file [vatom.c](#).

7.16.4.23 Vatom_setResName()

```
VEXTERNC void Vatom_setResName (
    Vatom * thee,
    char resName[VMAX_RECLEN] )
```

Set residue name.

Author

Jason Wagoner

Parameters

<i>thee</i>	Vatom object
<i>resName</i>	Residue Name

Definition at line 192 of file [vatom.c](#).

7.17 Vcap class

Collection of routines which cap certain exponential and hyperbolic functions.

Files

- file [vcap.c](#)
Class Vcap methods.
- file [vcap.h](#)
Contains declarations for class Vcap.

Macros

- #define [EXPMAX](#) 85.00
Maximum argument for exp(), sinh(), or cosh()
- #define [EXPMIN](#) -85.00
Minimum argument for exp(), sinh(), or cosh()

Functions

- VEXTERNC double [Vcap_exp](#) (double x, int *ichop)
Provide a capped exp() function.
- VEXTERNC double [Vcap_sinh](#) (double x, int *ichop)
Provide a capped sinh() function.
- VEXTERNC double [Vcap_cosh](#) (double x, int *ichop)
Provide a capped cosh() function.

7.17.1 Detailed Description

Collection of routines which cap certain exponential and hyperbolic functions.

Note

These routines are based on FORTRAN code by Mike Holst

7.17.2 Macro Definition Documentation

7.17.2.1 EXPMAX

```
#define EXPMAX 85.00
```

Maximum argument for exp(), sinh(), or cosh()

Definition at line 72 of file [vcap.h](#).

7.17.2.2 EXPMIN

```
#define EXPMIN -85.00
```

Minimum argument for exp(), sinh(), or cosh()

Definition at line 77 of file [vcap.h](#).

7.17.3 Function Documentation

7.17.3.1 Vcap_cosh()

```
VEXTERNC double Vcap_cosh (
    double x,
    int * ichop )
```

Provide a capped cosh() function.

If the argument x of Vcap_cosh() exceeds EXPMAX or EXPMIN, then we return cosh(EXPMAX) or cosh(EXPMIN) rather than cosh(x).

Note

Original FORTRAN routine from PMG library by Mike Holst Original notes: to control overflow in the hyperbolic and exp functions, note that the following are the argument limits of the various functions on various machines after which overflow occurs: Convex C240, Sun 3/60, Sun SPARC, IBM RS/6000: sinh, cosh, exp: maximal argument (abs value) = 88.0d0 dsinh, dcosh, dexp: maximal argument (abs value) = 709.0d0

Author

Nathan Baker (based on FORTRAN code by Mike Holst)

Returns

cosh(x) or capped equivalent

Parameters

<i>x</i>	Argument to cosh()
<i>ichop</i>	Set to 1 if function capped, 0 otherwise

Definition at line 91 of file [vcap.c](#).

7.17.3.2 Vcap_exp()

```
VEXTERNC double Vcap_exp (
    double x,
    int * ichop )
```

Provide a capped exp() function.

If the argument x of Vcap_exp() exceeds EXPMAX or EXPMIN, then we return exp(EXPMAX) or exp(EXPMIN) rather than exp(x).

Note

Original FORTRAN routine from PMG library by Mike Holst Original notes: to control overflow in the hyperbolic and exp functions, note that the following are the argument limits of the various functions on various machines after which overflow occurs: Convex C240, Sun 3/60, Sun SPARC, IBM RS/6000: sinh, cosh, exp: maximal argument (abs value) = 88.0d0 dsinh, dcosh, dexp: maximal argument (abs value) = 709.0d0

Author

Nathan Baker (based on FORTRAN code by Mike Holst)

Returns

$\exp(x)$ or capped equivalent

Parameters

<i>x</i>	Argument to $\exp()$
<i>ichop</i>	Set to 1 if function capped, 0 otherwise

Definition at line 59 of file [vcap.c](#).

7.17.3.3 Vcap_sinh()

```

VEXTERNC double Vcap_sinh (
    double x,
    int * ichop )

```

Provide a capped $\sinh()$ function.

```

If the argument x of Vcap_sinh() exceeds EXPMAX or EXPMIN, then we
return sinh(EXPMAX) or sinh(EXPMIN) rather than sinh(x).

```

Note

Original FORTRAN routine from PMG library by Mike Holst Original notes: to control overflow in the hyperbolic and exp functions, note that the following are the argument limits of the various functions on various machines after which overflow occurs: Convex C240, Sun 3/60, Sun SPARC, IBM RS/6000: sinh, cosh, exp: maximal argument (abs value) = 88.0d0 dsinh, dcosh, dexp: maximal argument (abs value) = 709.0d0

Author

Nathan Baker (based on FORTRAN code by Mike Holst)

Returns

$\sinh(x)$ or capped equivalent

Parameters

<i>x</i>	Argument to $\sinh()$
<i>ichop</i>	Set to 1 if function capped, 0 otherwise

Definition at line 75 of file [vcap.c](#).

7.18 Vclist class

Atom cell list.

Files

- file [vclist.c](#)
Class Vclist methods.
- file [vclist.h](#)
Contains declarations for class Vclist.

Data Structures

- struct [sVclistCell](#)
Atom cell list cell.
- struct [sVclist](#)
Atom cell list.

Typedefs

- typedef struct [sVclistCell](#) [VclistCell](#)
Declaration of the VclistCell class as the VclistCell structure.
- typedef struct [sVclist](#) [Vclist](#)
Declaration of the Vclist class as the Vclist structure.

Enumerations

- enum [eVclist_DomainMode](#) { [CLIST_AUTO_DOMAIN](#) , [CLIST_MANUAL_DOMAIN](#) }
Atom cell list domain setup mode.

Functions

- VEXTERNC unsigned long int [Vclist_memChk](#) ([Vclist](#) *thee)
Get number of bytes in this object and its members.
- VEXTERNC double [Vclist_maxRadius](#) ([Vclist](#) *thee)
Get the max probe radius value (in Å) the cell list was constructed with.
- VEXTERNC [Vclist](#) * [Vclist_ctor](#) ([Valist](#) *alist, double max_radius, int npts[[VAPBS_DIM](#)], [Vclist_DomainMode](#) mode, double lower_corner[[VAPBS_DIM](#)], double upper_corner[[VAPBS_DIM](#)])
Construct the cell list object.
- VEXTERNC [Vrc_Codes](#) [Vclist_ctor2](#) ([Vclist](#) *thee, [Valist](#) *alist, double max_radius, int npts[[VAPBS_DIM](#)], [Vclist_DomainMode](#) mode, double lower_corner[[VAPBS_DIM](#)], double upper_corner[[VAPBS_DIM](#)])
FORTTRAN stub to construct the cell list object.
- VEXTERNC void [Vclist_dtor](#) ([Vclist](#) **thee)
Destroy object.
- VEXTERNC void [Vclist_dtor2](#) ([Vclist](#) *thee)
FORTTRAN stub to destroy object.
- VEXTERNC [VclistCell](#) * [Vclist_getCell](#) ([Vclist](#) *thee, double position[[VAPBS_DIM](#)])
Return cell corresponding to specified position or return VNULL.
- VEXTERNC [VclistCell](#) * [VclistCell_ctor](#) (int natoms)
Allocate and construct a cell list cell object.
- VEXTERNC [Vrc_Codes](#) [VclistCell_ctor2](#) ([VclistCell](#) *thee, int natoms)
Construct a cell list object.
- VEXTERNC void [VclistCell_dtor](#) ([VclistCell](#) **thee)
Destroy object.
- VEXTERNC void [VclistCell_dtor2](#) ([VclistCell](#) *thee)
FORTTRAN stub to destroy object.

7.18.1 Detailed Description

Atom cell list.

7.18.2 Typedef Documentation

7.18.2.1 Vclist

```
typedef struct sVclist Vclist
```

Declaration of the Vclist class as the Vclist structure.

Definition at line 136 of file [vclist.h](#).

7.18.2.2 VclistCell

```
typedef struct sVclistCell VclistCell
```

Declaration of the VclistCell class as the VclistCell structure.

Definition at line 110 of file [vclist.h](#).

7.18.3 Enumeration Type Documentation

7.18.3.1 eVclist_DomainMode

```
enum eVclist_DomainMode
```

Atom cell list domain setup mode.

Author

Nathan Baker

Enumerator

CLIST_AUTO_DOMAIN	Setup the cell list domain automatically to encompass the entire molecule
CLIST_MANUAL_DOMAIN	Specify the cell list domain manually through the constructor

Definition at line 82 of file [vclist.h](#).

7.18.4 Function Documentation

7.18.4.1 Vclist_ctor()

```
VEXTERNC Vclist * Vclist_ctor (
    Valist * alist,
    double max_radius,
    int npts[VAPBS_DIM],
    Vclist_DomainMode mode,
    double lower_corner[VAPBS_DIM],
    double upper_corner[VAPBS_DIM] )
```

Construct the cell list object.

Author

Nathan Baker

Returns

Newly allocated Vclist object

Parameters

<i>alist</i>	Molecule for cell list queries
<i>max_radius</i>	Max probe radius (Å) to be queried
<i>npts</i>	Number of in hash table points in each direction
<i>mode</i>	Mode to construct table
<i>lower_corner</i>	Hash table lower corner for manual construction (see mode variable); ignored otherwise
<i>upper_corner</i>	Hash table upper corner for manual construction (see mode variable); ignored otherwise

Definition at line 75 of file [vclist.c](#).

7.18.4.2 Vclist_ctor2()

```
VEXTERNC Vrc_Codes Vclist_ctor2 (
    Vclist * thee,
    Valist * alist,
    double max_radius,
    int npts[VAPBS_DIM],
    Vclist_DomainMode mode,
    double lower_corner[VAPBS_DIM],
    double upper_corner[VAPBS_DIM] )
```

FORTRAN stub to construct the cell list object.

Author

Nathan Baker, Yong Huang

Returns

Success enumeration

Parameters

<i>thee</i>	Memory for Vclist objet
<i>alist</i>	Molecule for cell list queries
<i>max_radius</i>	Max probe radius (Å) to be queried
<i>npts</i>	Number of in hash table points in each direction
<i>mode</i>	Mode to construct table
<i>lower_corner</i>	Hash table lower corner for manual construction (see mode variable); ignored otherwise
<i>upper_corner</i>	Hash table upper corner for manual construction (see mode variable); ignored otherwise

Definition at line 343 of file [vclist.c](#).

7.18.4.3 Vclist_dtor()

```
VEXTERNC void Vclist_dtor (
    Vclist ** thee )
```

Destroy object.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to memory location of object
-------------	--------------------------------------

Definition at line 397 of file [vclist.c](#).

7.18.4.4 Vclist_dtor2()

```
VEXTERNC void Vclist_dtor2 (  
    Vclist * thee )
```

FORTTRAN stub to destroy object.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to object
-------------	-------------------

Definition at line 408 of file [vclist.c](#).

7.18.4.5 Vclist_getCell()

```
VEXTERNC VclistCell * Vclist_getCell (  
    Vclist * thee,  
    double position[VAPBS_DIM] )
```

Return cell corresponding to specified position or return VNULL.

Author

Nathan Baker

Returns

Pointer to VclistCell object or VNULL if no cell available (away from molecule).

Parameters

<i>thee</i>	Pointer to Vclist cell list
<i>position</i>	Position to evaluate

Definition at line 423 of file [vclist.c](#).

7.18.4.6 Vclist_maxRadius()

```
VEXTERNC double Vclist_maxRadius (  
    Vclist * thee )
```

Get the max probe radius value (in A) the cell list was constructed with.

Author

Nathan Baker

Returns

Max probe radius (in Å)

Parameters

<i>thee</i>	Cell list object
-------------	------------------

Definition at line 68 of file [vclist.c](#).

7.18.4.7 Vclist_memChk()

```
VEXTERNC unsigned long int Vclist_memChk (  
    Vclist * thee )
```

Get number of bytes in this object and its members.

Author

Nathan Baker

Returns

Number of bytes allocated for object

Parameters

<i>thee</i>	Object for memory check
-------------	-------------------------

Definition at line 63 of file [vclist.c](#).

7.18.4.8 VclistCell_ctor()

```
VEXTERNC VclistCell * VclistCell_ctor (  
    int natoms )
```

Allocate and construct a cell list cell object.

Author

Nathan Baker

Returns

Pointer to newly-allocated and constructed object.

Parameters

<i>natoms</i>	Number of atoms associated with this cell
---------------	---

Definition at line 452 of file [vclist.c](#).

7.18.4.9 VclistCell_ctor2()

```
VEXTERNC Vrc_Codes VclistCell_ctor2 (  
    VclistCell * thee,
```

```
int natoms )
```

Construct a cell list object.

Author

Nathan Baker, Yong Huang

Returns

Success enumeration

Parameters

<i>thee</i>	Memory location for object
<i>natoms</i>	Number of atoms associated with this cell

Definition at line 464 of file [vclist.c](#).

7.18.4.10 VclistCell_dtor()

```
VEXTERNC void VclistCell_dtor (
    VclistCell ** thee )
```

Destroy object.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to memory location of object
-------------	--------------------------------------

Definition at line 486 of file [vclist.c](#).

7.18.4.11 VclistCell_dtor2()

```
VEXTERNC void VclistCell_dtor2 (
    VclistCell * thee )
```

FORTTRAN stub to destroy object.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to object
-------------	-------------------

Definition at line 497 of file [vclist.c](#).

7.19 Vgreen class

Provides capabilities for pointwise evaluation of free space Green's function for point charges in a uniform dielectric.

Files

- file [vgreen.c](#)
Class Vgreen methods.
- file [vgreen.h](#)
Contains declarations for class Vgreen.

Data Structures

- struct [sVgreen](#)
Contains public data members for Vgreen class/module.

Typedefs

- typedef struct [sVgreen](#) [Vgreen](#)
Declaration of the Vgreen class as the Vgreen structure.

Functions

- VEXTERNC [Valist](#) * [Vgreen_getValist](#) ([Vgreen](#) *thee)
Get the atom list associated with this Green's function object.
- VEXTERNC unsigned long int [Vgreen_memChk](#) ([Vgreen](#) *thee)
Return the memory used by this structure (and its contents) in bytes.
- VEXTERNC [Vgreen](#) * [Vgreen_ctor](#) ([Valist](#) *alist)
Construct the Green's function oracle.
- VEXTERNC int [Vgreen_ctor2](#) ([Vgreen](#) *thee, [Valist](#) *alist)
FORTTRAN stub to construct the Green's function oracle.
- VEXTERNC void [Vgreen_dtor](#) ([Vgreen](#) **thee)
Destruct the Green's function oracle.
- VEXTERNC void [Vgreen_dtor2](#) ([Vgreen](#) *thee)
FORTTRAN stub to destruct the Green's function oracle.
- VEXTERNC int [Vgreen_helmholtz](#) ([Vgreen](#) *thee, int npos, double *x, double *y, double *z, double *val, double kappa)
Get the Green's function for Helmholtz's equation integrated over the atomic point charges.
- VEXTERNC int [Vgreen_helmholtzD](#) ([Vgreen](#) *thee, int npos, double *x, double *y, double *z, double *gradx, double *grady, double *gradz, double kappa)
Get the gradient of Green's function for Helmholtz's equation integrated over the atomic point charges.
- VEXTERNC int [Vgreen_coulomb_direct](#) ([Vgreen](#) *thee, int npos, double *x, double *y, double *z, double *val)
Get the Coulomb's Law Green's function (solution to Laplace's equation) integrated over the atomic point charges using direct summation.
- VEXTERNC int [Vgreen_coulomb](#) ([Vgreen](#) *thee, int npos, double *x, double *y, double *z, double *val)
Get the Coulomb's Law Green's function (solution to Laplace's equation) integrated over the atomic point charges using direct summation or H. E. Johnston, R. Krasny FMM library (if available)
- VEXTERNC int [Vgreen_coulombD_direct](#) ([Vgreen](#) *thee, int npos, double *x, double *y, double *z, double *pot, double *gradx, double *grady, double *gradz)
Get gradient of the Coulomb's Law Green's function (solution to Laplace's equation) integrated over the atomic point charges using direct summation.
- VEXTERNC int [Vgreen_coulombD](#) ([Vgreen](#) *thee, int npos, double *x, double *y, double *z, double *pot, double *gradx, double *grady, double *gradz)
Get gradient of the Coulomb's Law Green's function (solution to Laplace's equation) integrated over the atomic point charges using either direct summation or H. E. Johnston/R. Krasny FMM library (if available)

7.19.1 Detailed Description

Provides capabilities for pointwise evaluation of free space Green's function for point charges in a uniform dielectric.

Note

Right now, these are very slow methods without any fast multipole acceleration.

Attention

```
*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
* Nathan A. Baker (nathan.baker@pnnl.gov)
* Pacific Northwest National Laboratory
*
* Additional contributing authors listed in the code documentation.
*
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* CONTRACT, STRICT LIABILITY, OR TORT (INCLUDING NEGLIGENCE OR OTHERWISE)
* ARISING IN ANY WAY OUT OF THE USE OF THIS SOFTWARE, EVEN IF ADVISED OF
* THE POSSIBILITY OF SUCH DAMAGE.
*
*
```

7.19.2 Typedef Documentation

7.19.2.1 Vgreen

```
typedef struct sVgreen Vgreen
```

Declaration of the Vgreen class as the Vgreen structure.

Definition at line 101 of file [vgreen.h](#).

7.19.3 Function Documentation

7.19.3.1 Vgreen_coulomb()

```

VEXTERNC int Vgreen_coulomb (
    Vgreen * thee,
    int npos,
    double * x,
    double * y,
    double * z,
    double * val )

```

Get the Coulomb's Law Green's function (solution to Laplace's equation) integrated over the atomic point charges using direct summation or H. E. Johnston, R. Krasny FMM library (if available)

Returns the potential ϕ defined by

$$\phi(r) = \sum_i \frac{q_i}{r_i}$$

where q_i is the atomic charge (in e) and r_i is the distance to the observation point r . The potential is scaled to units of V.

Author

Nathan Baker

Parameters

<i>thee</i>	Vgreen object
<i>npos</i>	The number of positions to evaluate
<i>x</i>	The npos x-coordinates
<i>y</i>	The npos y-coordinates
<i>z</i>	The npos z-coordinates
<i>val</i>	The npos values

Returns

1 if successful, 0 otherwise

Definition at line 258 of file [vgreen.c](#).

7.19.3.2 Vgreen_coulomb_direct()

```

VEXTERNC int Vgreen_coulomb_direct (
    Vgreen * thee,
    int npos,
    double * x,
    double * y,
    double * z,
    double * val )

```

Get the Coulomb's Law Green's function (solution to Laplace's equation) integrated over the atomic point charges using direct summation.

Returns the potential ϕ defined by

$$\phi(r) = \sum_i \frac{q_i}{r_i}$$

where q_i is the atomic charge (in e) and r_i is the distance to the observation point r . The potential is scaled to units of V.

Author

Nathan Baker

Parameters

<i>thee</i>	Vgreen object
<i>npos</i>	The number of positions to evaluate
<i>x</i>	The npos x-coordinates
<i>y</i>	The npos y-coordinates
<i>z</i>	The npos z-coordinates
<i>val</i>	The npos values

Returns

1 if successful, 0 otherwise

Definition at line 224 of file [vgreen.c](#).

7.19.3.3 Vgreen_coulombD()

```

VEXTERNC int Vgreen_coulombD (
    Vgreen * thee,
    int npos,
    double * x,
    double * y,
    double * z,
    double * pot,
    double * gradx,
    double * grady,
    double * gradz )

```

Get gradient of the Coulomb's Law Green's function (solution to Laplace's equation) integrated over the atomic point charges using either direct summation or H. E. Johnston/R. Krasny FMM library (if available)

Returns the field $\nabla\phi$ defined by

$$\nabla\phi(r) = \sum_i \frac{q_i}{r_i}$$

where q_i is the atomic charge (in e) and r_i is the distance to the observation point r . The field is scaled to units of V/Å.

Author

Nathan Baker

Parameters

<i>thee</i>	Vgreen object
<i>npos</i>	The number of positions to evaluate
<i>x</i>	The npos x-coordinates
<i>y</i>	The npos y-coordinates
<i>z</i>	The npos z-coordinates
<i>pot</i>	The npos potential values
<i>gradx</i>	The npos gradient x-components
<i>grady</i>	The npos gradient y-components
<i>gradz</i>	The npos gradient z-components

Returns

1 if successful, 0 otherwise

Definition at line 362 of file [vgreen.c](#).

7.19.3.4 Vgreen_coulombD_direct()

```

VEXTERNC int Vgreen_coulombD_direct (
    Vgreen * thee,
    int npos,
    double * x,
    double * y,
    double * z,
    double * pot,
    double * gradx,
    double * grady,
    double * gradz )

```

Get gradient of the Coulomb's Law Green's function (solution to Laplace's equation) integrated over the atomic point charges using direct summation.

Returns the field $\nabla\phi$ defined by

$$\nabla\phi(r) = \sum_i \frac{q_i}{r_i}$$

where q_i is the atomic charge (in e) and r_i is the distance to the observation point r . The field is scaled to units of V/Å.

Author

Nathan Baker

Parameters

<i>thee</i>	Vgreen object
<i>npos</i>	The number of positions to evaluate
<i>x</i>	The npos x-coordinates
<i>y</i>	The npos y-coordinates
<i>z</i>	The npos z-coordinates
<i>pot</i>	The npos potential values
<i>gradx</i>	The npos gradient x-components
<i>grady</i>	The npos gradient y-components
<i>gradz</i>	The npos gradient z-components

Returns

1 if successful, 0 otherwise

Definition at line 310 of file [vgreen.c](#).

7.19.3.5 Vgreen_ctor()

```

VEXTERNC Vgreen * Vgreen_ctor (
    Valist * alist )

```

Construct the Green's function oracle.

Author

Nathan Baker

Parameters

<i>alist</i>	Atom (charge) list associated with object
--------------	---

Returns

Pointer to newly allocated Green's function oracle

Definition at line 156 of file [vgreen.c](#).

7.19.3.6 Vgreen_ctor2()

```
VEXTERNC int Vgreen_ctor2 (  
    Vgreen * thee,  
    Valist * alist )
```

FORTRAN stub to construct the Green's function oracle.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to memory allocated for object
<i>alist</i>	Atom (charge) list associated with object

Returns

1 if successful, 0 otherwise

Definition at line 167 of file [vgreen.c](#).

7.19.3.7 Vgreen_dtor()

```
VEXTERNC void Vgreen_dtor (  
    Vgreen ** thee )
```

Destruct the Green's function oracle.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to memory location for object
-------------	---------------------------------------

Definition at line 192 of file [vgreen.c](#).

7.19.3.8 Vgreen_dtor2()

```
VEXTERNC void Vgreen_dtor2 (
```

```
Vgreen * thee )
```

FORTRAN stub to destruct the Green's function oracle.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to object
-------------	-------------------

Definition at line 200 of file [vgreen.c](#).

7.19.3.9 Vgreen_getValist()

```
VEXTERNC Valist * Vgreen_getValist (
    Vgreen * thee )
```

Get the atom list associated with this Green's function object.

Author

Nathan Baker

Parameters

<i>thee</i>	Vgreen object
-------------	---------------

Returns

Pointer to Valist object associated with this Green's function object

Definition at line 142 of file [vgreen.c](#).

7.19.3.10 Vgreen_helmholtz()

```
VEXTERNC int Vgreen_helmholtz (
    Vgreen * thee,
    int npos,
    double * x,
    double * y,
    double * z,
    double * val,
    double kappa )
```

Get the Green's function for Helmholtz's equation integrated over the atomic point charges.

Returns the potential ϕ defined by

$$\phi(r) = \sum_i \frac{q_i e^{-\kappa r_i}}{r_i}$$

where κ is the inverse screening length (in Å) q_i is the atomic charge (in e), and r_i is the distance from atom i to the observation point r . The potential is scaled to units of V.

Author

Nathan Baker

Bug Not implemented yet

Note

Not implemented yet

Parameters

<i>thee</i>	Vgreen object
<i>npos</i>	Number of positions to evaluate
<i>x</i>	The npos x-coordinates
<i>y</i>	The npos y-coordinates
<i>z</i>	The npos z-coordinates
<i>val</i>	The npos values
<i>kappa</i>	The value of κ (see above)

Returns

1 if successful, 0 otherwise

Definition at line 209 of file [vgreen.c](#).

7.19.3.11 Vgreen_helmholtzD()

```

VEXTERNC int Vgreen_helmholtzD (
    Vgreen * thee,
    int npos,
    double * x,
    double * y,
    double * z,
    double * gradx,
    double * grady,
    double * gradz,
    double kappa )

```

Get the gradient of Green's function for Helmholtz's equation integrated over the atomic point charges.

Returns the field $\nabla\phi$ defined by

$$\nabla\phi(r) = \nabla \sum_i \frac{q_i e^{-\kappa r_i}}{r_i}$$

where κ is the inverse screening length (in Å). q_i is the atomic charge (in e), and r_i is the distance from atom i to the observation point r . The potential is scaled to units of V/Å.

Author

Nathan Baker

Bug Not implemented yet

Note

Not implemented yet

Parameters

<i>thee</i>	Vgreen object
<i>npos</i>	The number of positions to evaluate

Parameters

<i>x</i>	The npos x-coordinates
<i>y</i>	The npos y-coordinates
<i>z</i>	The npos z-coordinates
<i>gradx</i>	The npos gradient x-components
<i>grady</i>	The npos gradient y-components
<i>gradz</i>	The npos gradient z-components
<i>kappa</i>	The value of κ (see above)

Returns

int 1 if successful, 0 otherwise

Definition at line 216 of file [vgreen.c](#).

7.19.3.12 Vgreen_memChk()

```

VEXTERNC unsigned long int Vgreen_memChk (
    Vgreen * thee )

```

Return the memory used by this structure (and its contents) in bytes.

Author

Nathan Baker

Parameters

<i>thee</i>	Vgreen object
-------------	---------------

Returns

The memory used by this structure and its contents in bytes

Definition at line 149 of file [vgreen.c](#).

7.20 Vhal class

A "class" which consists solely of macro definitions which are used by several other classes.

Files

- file [vhal.h](#)
Contains generic macro definitions for APBS.

Macros

- #define [APBS_TIMER_WALL_CLOCK](#) 26
APBS total execution timer ID.
- #define [APBS_TIMER_SETUP](#) 27
APBS setup timer ID.
- #define [APBS_TIMER_SOLVER](#) 28

- APBS solver timer ID.*

• #define **APBS_TIMER_ENERGY** 29
- APBS energy timer ID.*

• #define **APBS_TIMER_FORCE** 30
- APBS force timer ID.*

• #define **APBS_TIMER_TEMP1** 31
- APBS temp timer #1 ID.*

• #define **APBS_TIMER_TEMP2** 32
- APBS temp timer #2 ID.*

• #define **MAXMOL** 5
- The maximum number of molecules that can be involved in a single PBE calculation.*

• #define **MAXION** 10
- The maximum number of ion species that can be involved in a single PBE calculation.*

• #define **MAXFOCUS** 5
- The maximum number of times an MG calculation can be focused.*

• #define **VMGNLEV** 4
- Minimum number of levels in a multigrid calculations.*

• #define **VREDFRAC** 0.25
- Maximum reduction of grid spacing during a focusing calculation.*

• #define **VAPBS_NVS** 4
- Number of vertices per simplex (hard-coded to 3D)*

• #define **VAPBS_DIM** 3
- Our dimension.*

• #define **VAPBS_RIGHT** 0
- Face definition for a volume.*

• #define **VAPBS_FRONT** 1
- Face definition for a volume.*

• #define **VAPBS_UP** 2
- Face definition for a volume.*

• #define **VAPBS_LEFT** 3
- Face definition for a volume.*

• #define **VAPBS_BACK** 4
- Face definition for a volume.*

• #define **VAPBS_DOWN** 5
- Face definition for a volume.*

• #define **VPMGSMALL** 1e-12
- A small number used in Vpmg to decide if points are on/off grid-lines or non-zero (etc.)*

• #define **SINH_MIN** -85.0
- Used to set the min values acceptable for sinh chopping.*

• #define **SINH_MAX** 85.0
- Used to set the max values acceptable for sinh chopping.*

• #define **VF77_MANGLE**(name, NAME) name
- Name-mangling macro for using FORTRAN functions in C code.*

• #define **VFLOOR**(value) floor(value)
- Wrapped floor to fix floating point issues in the Intel compiler.*

• #define **VEMBED**(rctag)
- Allows embedding of RCS ID tags in object files.*

Typedefs

- typedef enum [eVhal_PBEType](#) [Vhal_PBEType](#)
Declaration of the Vhal_PBEType type as the Vhal_PBEType enum.
- typedef enum [eVhal_IPKEYType](#) [Vhal_IPKEYType](#)
Declaration of the Vhal_IPKEYType type as the Vhal_IPKEYType enum.
- typedef enum [eVhal_NONLINType](#) [Vhal_NONLINType](#)
Declaration of the Vhal_NONLINType type as the Vhal_NONLINType enum.
- typedef enum [eVoutput_Format](#) [Voutput_Format](#)
Declaration of the Voutput_Format type as the VOutput_Format enum.
- typedef enum [eVbcfl](#) [Vbcfl](#)
Declare Vbcfl type.

Enumerations

- enum [eVrc_Codes](#) { [VRC_WARNING](#) = -1 , [VRC_FAILURE](#) = 0 , [VRC_SUCCESS](#) = 1 }
Return code enumerations.
- enum [eVsol_Meth](#) {
[VSOL_CGMG](#) , [VSOL_Newton](#) , [VSOL_MG](#) , [VSOL_CG](#) ,
[VSOL_SOR](#) , [VSOL_RBGS](#) , [VSOL_WJ](#) , [VSOL_Richardson](#) ,
[VSOL_CGMGAqua](#) , [VSOL_NewtonAqua](#) }
Solution Method enumerations.
- enum [eVsurf_Meth](#) {
[VSM_MOL](#) = 0 , [VSM_MOLSMOOTH](#) = 1 , [VSM_SPLINE](#) = 2 , [VSM_SPLINE3](#) = 3 ,
[VSM_SPLINE4](#) = 4 }
Types of molecular surface definitions.
- enum [eVhal_PBEType](#) {
[PBE_LPBE](#) , [PBE_NPBE](#) , [PBE_LRPBE](#) , [PBE_NRPBE](#) ,
[PBE_SMPBE](#) }
Version of PBE to solve.
- enum [eVhal_IPKEYType](#) { [IPKEY_SMPBE](#) = -2 , [IPKEY_LPBE](#) , [IPKEY_NPBE](#) }
Type of ipkey to use for MG methods.
- enum [eVhal_NONLINType](#) {
[NONLIN_LPBE](#) = 0 , [NONLIN_NPBE](#) , [NONLIN_SMPBE](#) , [NONLIN_LPBEAQUA](#) ,
[NONLIN_NPBEAQUA](#) }
Type of nonlinear to use for MG methods.
- enum [eVoutput_Format](#) { [OUTPUT_NULL](#) , [OUTPUT_FLAT](#) }
Output file format.
- enum [eVbcfl](#) {
[BCFL_ZERO](#) = 0 , [BCFL_SDH](#) = 1 , [BCFL_MDH](#) = 2 , [BCFL_UNUSED](#) = 3 ,
[BCFL_FOCUS](#) = 4 , [BCFL_MEM](#) = 5 , [BCFL_MAP](#) = 6 }
Types of boundary conditions.
- enum [eVchrg_Meth](#) { [VCM_TRIL](#) = 0 , [VCM_BSPL2](#) = 1 , [VCM_BSPL4](#) = 2 }
Types of charge discretization methods.
- enum [eVchrg_Src](#) { [VCM_CHARGE](#) = 0 , [VCM_PERMANENT](#) = 1 , [VCM_INDUCED](#) = 2 , [VCM_NLINDUCED](#) = 3 }
Charge source.
- enum [eVdata_Type](#) {
[VDT_CHARGE](#) , [VDT_POT](#) , [VDT_ATOMPOT](#) , [VDT_SMOL](#) ,
[VDT_SSPL](#) , [VDT_VDW](#) , [VDT_IVDW](#) , [VDT_LAP](#) ,
[VDT_EDENS](#) , [VDT_NDENS](#) , [VDT_QDENS](#) , [VDT_DIELX](#) ,
[VDT_DIELY](#) , [VDT_DIELZ](#) , [VDT_KAPPA](#) }

Types of (scalar) data that can be written out of APBS.

- enum `eVdata_Format` {
 `VDF_DX` =0 , `VDF_UHBD` =1 , `VDF_AVS` =2 , `VDF_MCSF` =3 ,
 `VDF_GZ` =4 , `VDF_FLAT` =5 , `VDF_DXBIN` =6 }

Format of data for APBS I/O.

7.20.1 Detailed Description

A "class" which consists solely of macro definitions which are used by several other classes.

7.20.2 Macro Definition Documentation

7.20.2.1 APBS_TIMER_ENERGY

```
#define APBS_TIMER_ENERGY 29
```

APBS energy timer ID.
Definition at line 347 of file [vhal.h](#).

7.20.2.2 APBS_TIMER_FORCE

```
#define APBS_TIMER_FORCE 30
```

APBS force timer ID.
Definition at line 353 of file [vhal.h](#).

7.20.2.3 APBS_TIMER_SETUP

```
#define APBS_TIMER_SETUP 27
```

APBS setup timer ID.
Definition at line 335 of file [vhal.h](#).

7.20.2.4 APBS_TIMER_SOLVER

```
#define APBS_TIMER_SOLVER 28
```

APBS solver timer ID.
Definition at line 341 of file [vhal.h](#).

7.20.2.5 APBS_TIMER_TEMP1

```
#define APBS_TIMER_TEMP1 31
```

APBS temp timer #1 ID.
Definition at line 359 of file [vhal.h](#).

7.20.2.6 APBS_TIMER_TEMP2

```
#define APBS_TIMER_TEMP2 32
```

APBS temp timer #2 ID.
Definition at line 365 of file [vhal.h](#).

7.20.2.7 APBS_TIMER_WALL_CLOCK

```
#define APBS_TIMER_WALL_CLOCK 26
```

APBS total execution timer ID.
Definition at line 329 of file [vhal.h](#).

7.20.2.8 MAXFOCUS

```
#define MAXFOCUS 5
```

The maximum number of times an MG calculation can be focused.

Definition at line 382 of file [vhal.h](#).

7.20.2.9 MAXION

```
#define MAXION 10
```

The maximum number of ion species that can be involved in a single PBE calculation.

Definition at line 377 of file [vhal.h](#).

7.20.2.10 MAXMOL

```
#define MAXMOL 5
```

The maximum number of molecules that can be involved in a single PBE calculation.

Definition at line 371 of file [vhal.h](#).

7.20.2.11 SINH_MAX

```
#define SINH_MAX 85.0
```

Used to set the max values acceptable for sinh chopping.

Definition at line 456 of file [vhal.h](#).

7.20.2.12 SINH_MIN

```
#define SINH_MIN -85.0
```

Used to set the min values acceptable for sinh chopping.

Definition at line 450 of file [vhal.h](#).

7.20.2.13 VAPBS_BACK

```
#define VAPBS_BACK 4
```

Face definition for a volume.

Note

Consistent with PMG if RIGHT = EAST, BACK = SOUTH

Definition at line 432 of file [vhal.h](#).

7.20.2.14 VAPBS_DIM

```
#define VAPBS_DIM 3
```

Our dimension.

Definition at line 402 of file [vhal.h](#).

7.20.2.15 VAPBS_DOWN

```
#define VAPBS_DOWN 5
```

Face definition for a volume.

Note

Consistent with PMG if RIGHT = EAST, BACK = SOUTH

Definition at line 438 of file [vhal.h](#).

7.20.2.16 VAPBS_FRONT

```
#define VAPBS_FRONT 1
```

Face definition for a volume.

Note

Consistent with PMG if RIGHT = EAST, BACK = SOUTH

Definition at line 414 of file [vhal.h](#).

7.20.2.17 VAPBS_LEFT

```
#define VAPBS_LEFT 3
```

Face definition for a volume.

Note

Consistent with PMG if RIGHT = EAST, BACK = SOUTH

Definition at line 426 of file [vhal.h](#).

7.20.2.18 VAPBS_NVS

```
#define VAPBS_NVS 4
```

Number of vertices per simplex (hard-coded to 3D)

Definition at line 397 of file [vhal.h](#).

7.20.2.19 VAPBS_RIGHT

```
#define VAPBS_RIGHT 0
```

Face definition for a volume.

Note

Consistent with PMG if RIGHT = EAST, BACK = SOUTH

Definition at line 408 of file [vhal.h](#).

7.20.2.20 VAPBS_UP

```
#define VAPBS_UP 2
```

Face definition for a volume.

Note

Consistent with PMG if RIGHT = EAST, BACK = SOUTH

Definition at line 420 of file [vhal.h](#).

7.20.2.21 VEMBED

```
#define VEMBED(  
    rctag )
```

Value:

```
VPPRIVATE const char* rctag; \  
static void* use_rcsid=(0 ? &use_rcsid : (void*)&rcsid);
```

Allows embedding of RCS ID tags in object files.

Author

Mike Holst

Definition at line 556 of file [vhal.h](#).

7.20.2.22 VF77_MANGLE

```
#define VF77_MANGLE(
    name,
    NAME ) name
```

Name-mangling macro for using FORTRAN functions in C code.

Definition at line 532 of file [vhal.h](#).

7.20.2.23 VFLOOR

```
#define VFLOOR(
    value ) floor(value)
```

Wrapped floor to fix floating point issues in the Intel compiler.

Author

Todd Dolinsky

Definition at line 547 of file [vhal.h](#).

7.20.2.24 VMGNLEV

```
#define VMGNLEV 4
```

Minimum number of levels in a multigrid calculations.

Definition at line 387 of file [vhal.h](#).

7.20.2.25 VPMGSMALL

```
#define VPMGSMALL 1e-12
```

A small number used in Vpmg to decide if points are on/off grid-lines or non-zero (etc.)

Definition at line 444 of file [vhal.h](#).

7.20.2.26 VREDFRAC

```
#define VREDFRAC 0.25
```

Maximum reduction of grid spacing during a focusing calculation.

Definition at line 392 of file [vhal.h](#).

7.20.3 Typedef Documentation

7.20.3.1 Vbcfl

```
typedef enum eVbcfl Vbcfl
```

Declare Vbcfl type.

Definition at line 223 of file [vhal.h](#).

7.20.3.2 Vhal_IPKEYType

```
typedef enum eVhal_IPKEYType Vhal_IPKEYType
```

Declaration of the Vhal_IPKEYType type as the Vhal_IPKEYType enum.

Definition at line 167 of file [vhal.h](#).

7.20.3.3 Vhal_NONLINType

```
typedef enum eVhal_NONLINType Vhal_NONLINType
```

Declaration of the Vhal_NONLINType type as the Vhal_NONLINType enum.

Definition at line 185 of file [vhal.h](#).

7.20.3.4 Vhal_PBEType

```
typedef enum eVhal_PBEType Vhal_PBEType
```

Declaration of the Vhal_PBEType type as the Vhal_PBEType enum.

Definition at line 151 of file [vhal.h](#).

7.20.3.5 Voutput_Format

```
typedef enum eVoutput_Format Voutput_Format
```

Declaration of the Voutput_Format type as the VOutput_Format enum.

Definition at line 200 of file [vhal.h](#).

7.20.4 Enumeration Type Documentation

7.20.4.1 eVbcfl

```
enum eVbcfl
```

Types of boundary conditions.

Author

Nathan Baker

Enumerator

BCFL_ZERO	Zero Dirichlet boundary conditions
BCFL_SDH	Single-sphere Debye-Huckel Dirichlet boundary condition
BCFL_MDH	Multiple-sphere Debye-Huckel Dirichlet boundary condition
BCFL_UNUSED	Unused boundary condition method (placeholder)
BCFL_FOCUS	Focusing Dirichlet boundary condition
BCFL_MEM	Focusing membrane boundary condition
BCFL_MAP	Skip first level of focusing use an external map

Definition at line 207 of file [vhal.h](#).

7.20.4.2 eVchrg_Meth

```
enum eVchrg_Meth
```

Types of charge discretization methods.

Author

Nathan Baker

Enumerator

VCM_TRIL	Trilinear interpolation of charge to 8 nearest grid points. The traditional method; not particularly good to use with PBE forces.
VCM_BSPL2	Cubic B-spline across nearest- and next-nearest-neighbors. Mainly for use in grid-sensitive applications (such as force calculations).
VCM_BSPL4	5th order B-spline for AMOEBA permanent multipoles.

Definition at line 230 of file [vhal.h](#).

7.20.4.3 eVchrg_Src

enum [eVchrg_Src](#)

Charge source.

Author

Michael Schnieders

Enumerator

VCM_CHARGE	Partial Charge source distribution
VCM_PERMANENT	Permanent Multipole source distribution
VCM_INDUCED	Induced Dipole source distribution
VCM_NLINDUCED	NL Induced Dipole source distribution

Definition at line [251](#) of file [vhal.h](#).

7.20.4.4 eVdata_Format

enum [eVdata_Format](#)

Format of data for APBS I/O.

Author

Nathan Baker

Enumerator

VDF_DX	OpenDX (Data Explorer) format
VDF_UHBD	UHBD format
VDF_AVS	AVS UCD format
VDF_MCSF	FEtk MC Simplex Format (MCSF)
VDF_GZ	Binary file (GZip)
VDF_FLAT	Write flat file
VDF_DXBIN	OpendDX (Data Explorer) binary format

Definition at line [309](#) of file [vhal.h](#).

7.20.4.5 eVdata_Type

enum [eVdata_Type](#)

Types of (scalar) data that can be written out of APBS.

Author

Nathan Baker

Enumerator

VDT_CHARGE	Charge distribution (e)
VDT_POT	Potential (kT/e)
VDT_ATOMPOT	Atom potential (kT/e)

Enumerator

VDT_SMOL	Solvent accessibility defined by molecular/Connolly surface definition (1 = accessible, 0 = inaccessible)
VDT_SSPL	Spline-based solvent accessibility (1 = accessible, 0 = inaccessible)
VDT_VDW	van der Waals-based accessibility (1 = accessible, 0 = inaccessible)
VDT_IVDW	Ion accessibility/inflated van der Waals (1 = accessible, 0 = inaccessible)
VDT_LAP	Laplacian of potential ($kT/e/A^2$)
VDT_EDENS	Energy density $\epsilon(\nabla u)^2$, where u is potential ($kT/e/A^2$)
VDT_NDENS	Ion number density $\sum c_i \exp(-q_i u)^2$, where u is potential (output in M)
VDT_QDENS	Ion charge density $\sum q_i c_i \exp(-q_i u)^2$, where u is potential (output in $e_c M$)
VDT_DIELX	Dielectric x-shifted map as calculated with the currently specified scheme (dimensionless)
VDT_DIELY	Dielectric y-shifted map as calculated with the currently specified scheme (dimensionless)
VDT_DIELZ	Dielectric z-shifted map as calculated with the currently specified scheme (dimensionless)
VDT_KAPPA	Kappa map as calculated with the currently specified scheme ($^{-3}$)

Definition at line 269 of file [vhal.h](#).

7.20.4.6 eVhal_IPKEYType

enum [eVhal_IPKEYType](#)

Type of ipkey to use for MG methods.

Enumerator

IPKEY_SMPBE	SMPBE ipkey
IPKEY_LPBE	LPBE ipkey
IPKEY_NPBE	NPBE ipkey

Definition at line 157 of file [vhal.h](#).

7.20.4.7 eVhal_NONLINType

enum [eVhal_NONLINType](#)

Type of nonlinear to use for MG methods.

Definition at line 173 of file [vhal.h](#).

7.20.4.8 eVhal_PBEType

enum [eVhal_PBEType](#)

Version of PBE to solve.

Enumerator

PBE_LPBE	Traditional Poisson-Boltzmann equation, linearized
PBE_NPBE	Traditional Poisson-Boltzmann equation, full
PBE_LRPBE	Regularized Poisson-Boltzmann equation, linearized
PBE_SMPBE	< Regularized Poisson-Boltzmann equation, full SM PBE

Definition at line 139 of file [vhal.h](#).

7.20.4.9 eVoutput_Format

enum [eVoutput_Format](#)

Output file format.

Enumerator

OUTPUT_NULL	No output
OUTPUT_FLAT	Output in flat-file format

Definition at line 191 of file [vhal.h](#).

7.20.4.10 eVrc_Codes

enum [eVrc_Codes](#)

Return code enumerations.

Author

David Gohara

Note

Note that the enumerated values are opposite the standard for FAILURE and SUCCESS

Enumerator

VRC_FAILURE	A non-fatal error
VRC_SUCCESS	A fatal error

Definition at line 66 of file [vhal.h](#).

7.20.4.11 eVsol_Meth

enum [eVsol_Meth](#)

Solution Method enumerations.

Author

David Gohara

Note

Note that the enumerated values are opposite the standard for FAILURE and SUCCESS

Definition at line 81 of file [vhal.h](#).

7.20.4.12 eVsurf_Meth

enum [eVsurf_Meth](#)

Types of molecular surface definitions.

Author

Nathan Baker

Enumerator

VSM_MOL	Ion accessibility is defined using inflated van der Waals radii, the dielectric coefficient () is defined using the molecular (Conolly) surface definition without smoothing
VSM_MOLSMOOTH	As VSM_MOL but with a simple harmonic average smoothing
VSM_SPLINE	Spline-based surface definitions. This is primarily for use with force calculations, since it requires substantial reparameterization of radii. This is based on the work of Im et al, Comp. Phys. Comm. 111 , (1998) and uses a cubic spline to define a smoothly varying characteristic function for the surface-based parameters. Ion accessibility is defined using inflated van der Waals radii with the spline function and the dielectric coefficient is defined using the standard van der Waals radii with the spline function.
VSM_SPLINE3	A 5th order polynomial spline is used to create a smoothly varying characteristic function (continuity through 2nd derivatives) for surface based paramters.
VSM_SPLINE4	A 7th order polynomial spline is used to create a smoothly varying characteristic function (continuity through 3rd derivatives) for surface based paramters.

Definition at line 102 of file [vhal.h](#).

7.21 Matrix wrapper class

A header for including data wrapping matrices.

Files

- file [vmatrix.h](#)
Contains inclusions for matrix data wrappers.

7.21.1 Detailed Description

A header for including data wrapping matrices.

7.22 Vparam class

Reads and assigns charge/radii parameters.

Files

- file [vparam.c](#)
Class [Vparam](#) methods.
- file [vparam.h](#)
Contains declarations for class [Vparam](#).

Data Structures

- struct [sVparam_AtomData](#)
AtomData sub-class; stores atom data.
- struct [Vparam_ResData](#)
ResData sub-class; stores residue data.
- struct [Vparam](#)
Reads and assigns charge/radii parameters.

Typedefs

- typedef struct [sVparam_AtomData](#) [Vparam_AtomData](#)
Declaration of the [Vparam_AtomData](#) class as the [sVparam_AtomData](#) structure.

Functions

- VPRIVATE int [readFlatFileLine](#) (Vio *sock, [Vparam_AtomData](#) *atom)
Read a single line of the flat file database.
- VPRIVATE int [readXMLFileAtom](#) (Vio *sock, [Vparam_AtomData](#) *atom)
Read atom information from an XML file.
- VEXTERNC unsigned long int [Vparam_memChk](#) ([Vparam](#) *thee)
Get number of bytes in this object and its members.
- VEXTERNC [Vparam_AtomData](#) * [Vparam_AtomData_ctor](#) ()
Construct the object.
- VEXTERNC int [Vparam_AtomData_ctor2](#) ([Vparam_AtomData](#) *thee)
FORTTRAN stub to construct the object.
- VEXTERNC void [Vparam_AtomData_dtor](#) ([Vparam_AtomData](#) **thee)
Destroy object.
- VEXTERNC void [Vparam_AtomData_dtor2](#) ([Vparam_AtomData](#) *thee)
FORTTRAN stub to destroy object.
- VEXTERNC void [Vparam_AtomData_copyTo](#) ([Vparam_AtomData](#) *thee, [Vparam_AtomData](#) *dest)
Copy current atom object to destination.
- VEXTERNC void [Vparam_ResData_copyTo](#) ([Vparam_ResData](#) *thee, [Vparam_ResData](#) *dest)
Copy current residue object to destination.
- VEXTERNC void [Vparam_AtomData_copyFrom](#) ([Vparam_AtomData](#) *thee, [Vparam_AtomData](#) *src)
Copy current atom object from another.
- VEXTERNC [Vparam_ResData](#) * [Vparam_ResData_ctor](#) (Vmem *mem)
Construct the object.
- VEXTERNC int [Vparam_ResData_ctor2](#) ([Vparam_ResData](#) *thee, Vmem *mem)
FORTTRAN stub to construct the object.
- VEXTERNC void [Vparam_ResData_dtor](#) ([Vparam_ResData](#) **thee)
Destroy object.
- VEXTERNC void [Vparam_ResData_dtor2](#) ([Vparam_ResData](#) *thee)
FORTTRAN stub to destroy object.
- VEXTERNC [Vparam](#) * [Vparam_ctor](#) ()
Construct the object.
- VEXTERNC int [Vparam_ctor2](#) ([Vparam](#) *thee)
FORTTRAN stub to construct the object.
- VEXTERNC void [Vparam_dtor](#) ([Vparam](#) **thee)
Destroy object.
- VEXTERNC void [Vparam_dtor2](#) ([Vparam](#) *thee)
FORTTRAN stub to destroy object.
- VEXTERNC [Vparam_ResData](#) * [Vparam_getResData](#) ([Vparam](#) *thee, char resName[VMAX_ARGLEN])
Get residue data.
- VEXTERNC [Vparam_AtomData](#) * [Vparam_getAtomData](#) ([Vparam](#) *thee, char resName[VMAX_ARGLEN], char atomName[VMAX_ARGLEN])
Get atom data.

- VEXTERNC int [Vparam_readFlatFile](#) ([Vparam](#) *thee, const char *iodev, const char *iofmt, const char *thost, const char *fname)

Read a flat-file format parameter database.

- VEXTERNC int [Vparam_readXMLFile](#) ([Vparam](#) *thee, const char *iodev, const char *iofmt, const char *thost, const char *fname)

Read an XML format parameter database.

Variables

- VPRIVATE char * [MCwhiteChars](#) = " =,;\t\n\r"
Whitespace characters for socket reads.
- VPRIVATE char * [MCcommChars](#) = "#%"
Comment characters for socket reads.
- VPRIVATE char * [MCxmlwhiteChars](#) = " =,;\t\n\r<>"
Whitespace characters for XML socket reads.

7.22.1 Detailed Description

Reads and assigns charge/radii parameters.

7.22.2 Typedef Documentation

7.22.2.1 Vparam_AtomData

typedef struct [sVparam_AtomData](#) [Vparam_AtomData](#)

Declaration of the Vparam_AtomData class as the [sVparam_AtomData](#) structure.

Definition at line 106 of file [vparam.h](#).

7.22.3 Function Documentation

7.22.3.1 readFlatFileLine()

```
VPRIVATE int readFlatFileLine (
    Vio * sock,
    Vparam\_AtomData * atom )
```

Read a single line of the flat file database.

Author

Nathan Baker

Parameters

<i>sock</i>	Socket ready for reading
<i>atom</i>	Atom to hold parsed data

Returns

1 if successful, 0 otherwise

Definition at line 691 of file [vparam.c](#).

7.22.3.2 readXMLFileAtom()

```
VPRIVATE int readXMLFileAtom (
```

```
Vio * sock,  
Vparam_AtomData * atom )
```

Read atom information from an XML file.

Author

Todd Dolinsky

Parameters

<i>sock</i>	Socket ready for reading
<i>atom</i>	Atom to hold parsed data

Returns

1 if successful, 0 otherwise

Definition at line 610 of file [vparam.c](#).

7.22.3.3 Vparam_AtomData_copyFrom()

```
VEXTERNC void Vparam_AtomData_copyFrom (  
    Vparam_AtomData * thee,  
    Vparam_AtomData * src )
```

Copy current atom object from another.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to destination object
<i>src</i>	Pointer to source object

Definition at line 607 of file [vparam.c](#).

7.22.3.4 Vparam_AtomData_copyTo()

```
VEXTERNC void Vparam_AtomData_copyTo (  
    Vparam_AtomData * thee,  
    Vparam_AtomData * dest )
```

Copy current atom object to destination.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to source object
<i>dest</i>	Pointer to destination object

Definition at line 571 of file [vparam.c](#).

7.22.3.5 Vparam_AtomData_ctor()

```
VEXTERNC Vparam_AtomData * Vparam_AtomData_ctor ( )
```

Construct the object.

Author

Nathan Baker

Returns

Newly allocated object

Definition at line 109 of file [vparam.c](#).

7.22.3.6 Vparam_AtomData_ctor2()

```
VEXTERNC int Vparam_AtomData_ctor2 (
    Vparam_AtomData * thee )
```

FORTTRAN stub to construct the object.

Author

Nathan Baker

Parameters

<i>thee</i>	Allocated memory
-------------	------------------

Returns

1 if successful, 0 otherwise

Definition at line 121 of file [vparam.c](#).

7.22.3.7 Vparam_AtomData_dtor()

```
VEXTERNC void Vparam_AtomData_dtor (
    Vparam_AtomData ** thee )
```

Destroy object.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to memory location of object
-------------	--------------------------------------

Definition at line 123 of file [vparam.c](#).

7.22.3.8 Vparam_AtomData_dtor2()

```
VEXTERNC void Vparam_AtomData_dtor2 (
    Vparam_AtomData * thee )
```

FORTTRAN stub to destroy object.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to object
-------------	-------------------

Definition at line 133 of file [vparam.c](#).

7.22.3.9 Vparam_ctor()

```
VEXTERNC Vparam * Vparam_ctor ( )
```

Construct the object.

Author

Nathan Baker

Returns

Newly allocated [Vparam](#) object

Definition at line 181 of file [vparam.c](#).

7.22.3.10 Vparam_ctor2()

```
VEXTERNC int Vparam_ctor2 (
    Vparam * thee )
```

FORTTRAN stub to construct the object.

Author

Nathan Baker

Parameters

<i>thee</i>	Allocated Vparam memory
-------------	---

Returns

1 if successful, 0 otherwise

Definition at line 193 of file [vparam.c](#).

7.22.3.11 Vparam_dtor()

```
VEXTERNC void Vparam_dtor (
    Vparam ** thee )
```

Destroy object.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to memory location of object
-------------	--------------------------------------

Definition at line 213 of file [vparam.c](#).

7.22.3.12 Vparam_dtor2()

```
VEXTERNC void Vparam_dtor2 (  
    Vparam * thee )
```

FORTTRAN stub to destroy object.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to object
-------------	-------------------

Definition at line 223 of file [vparam.c](#).

7.22.3.13 Vparam_getAtomData()

```
VEXTERNC Vparam_AtomData * Vparam_getAtomData (  
    Vparam * thee,  
    char resName[VMAX_ARGLLEN],  
    char atomName[VMAX_ARGLLEN] )
```

Get atom data.

Author

Nathan Baker

Parameters

<i>thee</i>	Vparam object
<i>resName</i>	Residue name
<i>atomName</i>	Atom name

Returns

Pointer to the desired atom object or VNULL if residue not found

Note

Some method to initialize the database must be called before this method (e.g.,

See also

[Vparam_readFlatFile\(\)](#)

Definition at line 267 of file [vparam.c](#).

7.22.3.14 Vparam_getResData()

```
VEXTERNC Vparam_ResData * Vparam_getResData (
    Vparam * thee,
    char resName[VMAX_ARGLLEN] )
```

Get residue data.

Author

Nathan Baker

Parameters

<i>thee</i>	Vparam object
<i>resName</i>	Residue name

Returns

Pointer to the desired residue object or VNULL if residue not found

Note

Some method to initialize the database must be called before this method (e.g.,

See also

[Vparam_readFlatFile\(\)](#)

Definition at line 241 of file [vparam.c](#).

7.22.3.15 Vparam_memChk()

```
VEXTERNC unsigned long int Vparam_memChk (
    Vparam * thee )
```

Get number of bytes in this object and its members.

Author

Nathan Baker

Parameters

<i>thee</i>	Vparam object
-------------	---------------

Returns

Number of bytes allocated for object

Definition at line 102 of file [vparam.c](#).

7.22.3.16 Vparam_readFlatFile()

```
VEXTERNC int Vparam_readFlatFile (
    Vparam * thee,
    const char * iodev,
```



```
const char * iofmt,
const char * thost,
const char * fname )
```

Read a flat-file format parameter database.

Author

Nathan Baker

Parameters

<i>thee</i>	Vparam object
<i>iodev</i>	Input device type (FILE/BUFF/UNIX/INET)
<i>iofmt</i>	Input device format (ASCII/XDR)
<i>thost</i>	Input hostname (for sockets)
<i>fname</i>	Input FILE/BUFF/UNIX/INET name (see note below for format)

Returns

1 if successful, 0 otherwise

Note

The database file should have the following format:

```
RESIDUE ATOM CHARGE RADIUS EPSILON
```

where RESIDUE is the residue name string, ATOM is the atom name string, CHARGE is the charge in e, RADIUS is the van der Waals radius (σ_i) in Å, and EPSILON is the van der Waals well-depth (ϵ_i) in kJ/mol. See the [Vparam](#) structure documentation for the precise definitions of σ_i and ϵ_i .

ASCII-format flat files are provided with the APBS source code:

tools/conversion/vparam-amber-parm94.dat AMBER parm94 parameters

tools/conversion/vparam-charmm-par_all27.dat CHARMM par_all27_prot_na parameters

Definition at line [445](#) of file [vparam.c](#).

7.22.3.17 Vparam_readXMLFile()

```
VEXTERNC int Vparam_readXMLFile (
    Vparam * thee,
    const char * iodev,
    const char * iofmt,
    const char * thost,
    const char * fname )
```

Read an XML format parameter database.

Author

Todd Dolinsky

Parameters

<i>thee</i>	Vparam object
-------------	-------------------------------

Parameters

<i>iodev</i>	Input device type (FILE/BUFF/UNIX/INET)
<i>iofmt</i>	Input device format (ASCII/XDR)
<i>thost</i>	Input hostname (for sockets)
<i>fname</i>	Input FILE/BUFF/UNIX/INET name

Returns

1 if successful, 0 otherwise

Definition at line 306 of file [vparam.c](#).

7.22.3.18 Vparam_ResData_copyTo()

```
VEXTERNC void Vparam_ResData_copyTo (
    Vparam_ResData * thee,
    Vparam_ResData * dest )
```

Copy current residue object to destination.

Author

Todd Dolinsky

Parameters

<i>thee</i>	Pointer to source object
<i>dest</i>	Pointer to destination object

Definition at line 585 of file [vparam.c](#).

7.22.3.19 Vparam_ResData_ctor()

```
VEXTERNC Vparam_ResData * Vparam_ResData_ctor (
    Vmem * mem )
```

Construct the object.

Author

Nathan Baker

Parameters

<i>mem</i>	Memory object of Vparam master class
------------	--

Returns

Newly allocated object

Definition at line 135 of file [vparam.c](#).

7.22.3.20 Vparam_ResData_ctor2()

```
VEXTERNC int Vparam_ResData_ctor2 (
```

```
Vparam_ResData * thee,
Vmem * mem )
```

FORTTRAN stub to construct the object.

Author

Nathan Baker

Parameters

<i>thee</i>	Allocated memory
<i>mem</i>	Memory object of Vparam master class

Returns

1 if successful, 0 otherwise

Definition at line [147](#) of file [vparam.c](#).

7.22.3.21 Vparam_ResData_dtor()

```
VEEXTERNC void Vparam_ResData_dtor (
    Vparam_ResData ** thee )
```

Destroy object.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to memory location of object
-------------	--------------------------------------

Definition at line [160](#) of file [vparam.c](#).

7.22.3.22 Vparam_ResData_dtor2()

```
VEEXTERNC void Vparam_ResData_dtor2 (
    Vparam_ResData * thee )
```

FORTTRAN stub to destroy object.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to object
-------------	-------------------

Definition at line [170](#) of file [vparam.c](#).

7.22.4 Variable Documentation

7.22.4.1 MCcommChars

```
VPRIVATE char* MCcommChars = "#%"
```

Comment characters for socket reads.

Definition at line 71 of file [vparam.c](#).

7.22.4.2 MCwhiteChars

```
VPRIVATE char* MCwhiteChars = " =,;\t\n\r"
```

Whitespace characters for socket reads.

Definition at line 65 of file [vparam.c](#).

7.22.4.3 MCxmlwhiteChars

```
VPRIVATE char* MCxmlwhiteChars = " =,;\t\n\r<>"
```

Whitespace characters for XML socket reads.

Definition at line 77 of file [vparam.c](#).

7.23 Vpbe class

The Poisson-Boltzmann master class.

Files

- file [vpbe.c](#)
Class Vpbe methods.
- file [vpbe.h](#)
Contains declarations for class Vpbe.

Data Structures

- struct [sVpbe](#)
Contains public data members for Vpbe class/module.

Typedefs

- typedef struct [sVpbe](#) [Vpbe](#)
Declaration of the Vpbe class as the Vpbe structure.

Functions

- VEXTERNC [Valist](#) * [Vpbe_getValist](#) ([Vpbe](#) *thee)
Get atom list.
- VEXTERNC [Vacc](#) * [Vpbe_getVacc](#) ([Vpbe](#) *thee)
Get accessibility oracle.
- VEXTERNC double [Vpbe_getBulkIonicStrength](#) ([Vpbe](#) *thee)
Get bulk ionic strength.
- VEXTERNC double [Vpbe_getMaxIonRadius](#) ([Vpbe](#) *thee)
Get maximum radius of ion species.
- VEXTERNC double [Vpbe_getTemperature](#) ([Vpbe](#) *thee)
Get temperature.

- VEXTERNC double [Vpbe_getSoluteDiel](#) (Vpbe *thee)
Get solute dielectric constant.
- VEXTERNC double [Vpbe_getGamma](#) (Vpbe *thee)
Get apolar coefficient.
- VEXTERNC double [Vpbe_getSoluteRadius](#) (Vpbe *thee)
Get sphere radius which bounds biomolecule.
- VEXTERNC double [Vpbe_getSoluteXlen](#) (Vpbe *thee)
Get length of solute in x dimension.
- VEXTERNC double [Vpbe_getSoluteYlen](#) (Vpbe *thee)
Get length of solute in y dimension.
- VEXTERNC double [Vpbe_getSoluteZlen](#) (Vpbe *thee)
Get length of solute in z dimension.
- VEXTERNC double * [Vpbe_getSoluteCenter](#) (Vpbe *thee)
Get coordinates of solute center.
- VEXTERNC double [Vpbe_getSoluteCharge](#) (Vpbe *thee)
Get total solute charge.
- VEXTERNC double [Vpbe_getSolventDiel](#) (Vpbe *thee)
Get solvent dielectric constant.
- VEXTERNC double [Vpbe_getSolventRadius](#) (Vpbe *thee)
Get solvent molecule radius.
- VEXTERNC double [Vpbe_getXkappa](#) (Vpbe *thee)
Get Debye-Huckel parameter.
- VEXTERNC double [Vpbe_getDeblen](#) (Vpbe *thee)
Get Debye-Huckel screening length.
- VEXTERNC double [Vpbe_getZkappa2](#) (Vpbe *thee)
Get modified squared Debye-Huckel parameter.
- VEXTERNC double [Vpbe_getZmagic](#) (Vpbe *thee)
Get charge scaling factor.
- VEXTERNC double [Vpbe_getzmem](#) (Vpbe *thee)
Get z position of the membrane bottom.
- VEXTERNC double [Vpbe_getLmem](#) (Vpbe *thee)
Get length of the membrane (A)
aaauthor Michael Grabe.
- VEXTERNC double [Vpbe_getmembraneDiel](#) (Vpbe *thee)
Get membrane dielectric constant.
- VEXTERNC double [Vpbe_getmemv](#) (Vpbe *thee)
Get membrane potential (kT)
- VEXTERNC [Vpbe](#) * [Vpbe_ctor](#) (Valist *alist, int ionNum, double *ionConc, double *ionRadii, double *ionQ, double T, double soluteDiel, double solventDiel, double solventRadius, int focusFlag, double sdens, double z_↔mem, double L, double membraneDiel, double V)
Construct Vpbe object.
- VEXTERNC int [Vpbe_ctor2](#) (Vpbe *thee, Valist *alist, int ionNum, double *ionConc, double *ionRadii, double *ionQ, double T, double soluteDiel, double solventDiel, double solventRadius, int focusFlag, double sdens, double z_mem, double L, double membraneDiel, double V)
FORTTRAN stub to construct Vpbe objct.
- VEXTERNC int [Vpbe_getlons](#) (Vpbe *thee, int *nion, double ionConc[[MAXION](#)], double ionRadii[[MAXION](#)], double ionQ[[MAXION](#)])
Get information about the counterion species present.

- VEXTERNC void [Vpbe_dtor](#) ([Vpbe](#) **thee)
Object destructor.
- VEXTERNC void [Vpbe_dtor2](#) ([Vpbe](#) *thee)
FORTTRAN stub object destructor.
- VEXTERNC double [Vpbe_getCoulombEnergy1](#) ([Vpbe](#) *thee)
Calculate coulombic energy of set of charges.
- VEXTERNC unsigned long int [Vpbe_memChk](#) ([Vpbe](#) *thee)
Return the memory used by this structure (and its contents) in bytes.

7.23.1 Detailed Description

The Poisson-Boltzmann master class.

Contains objects and parameters used in every PBE calculation, regardless of method.

7.23.2 Typedef Documentation

7.23.2.1 Vpbe

```
typedef struct sVpbe Vpbe
```

Declaration of the Vpbe class as the Vpbe structure.

Definition at line 144 of file [vpbe.h](#).

7.23.3 Function Documentation

7.23.3.1 Vpbe_ctor()

```
VEXTERNC Vpbe * Vpbe_ctor (
    Valist * alist,
    int ionNum,
    double * ionConc,
    double * ionRadii,
    double * ionQ,
    double T,
    double soluteDiel,
    double solventDiel,
    double solventRadius,
    int focusFlag,
    double sdens,
    double z_mem,
    double L,
    double membraneDiel,
    double V )
```

Construct Vpbe object.

Author

Nathan Baker and Mike Holst and Michael Grabe

Note

This is partially based on some of Mike Holst's PMG code. Here are a few of the original function comments: kappa is defined as follows:

$$\kappa^2 = \frac{8\pi N_A e_c^2 I_s}{1000 \epsilon_w k_B T}$$

where the units are esu*esu/erg/mol. To obtain κ^{-2} , we multiply by 10^{-16} . Thus, in κ^{-2} , where k_B and e_c are in gaussian rather than mks units, the proper value for kappa is:

$$\kappa^2 = \frac{8\pi N_A e_c^2 I_s}{1000 \epsilon_w k_b T} \times 10^{-16}$$

and the factor of 10^{-16} results from converting cm^2 to angstroms^2 , noting that the 1000 in the denominator has converted m^3 to cm^3 , since the ionic strength I_s is assumed to have been provided in moles per liter, which is moles per 1000 cm^3 .

Returns

Pointer to newly allocated Vpbe object

Parameters

<i>alist</i>	Atom list
<i>ionNum</i>	Number of counterion species
<i>ionConc</i>	Array containing counterion concentrations (M)
<i>ionRadii</i>	Array containing counterion radii (A)
<i>ionQ</i>	Array containing counterion charges (e)
<i>T</i>	Temperature for Boltzmann distribution (K)
<i>soluteDiel</i>	Solute internal dielectric constant
<i>solventDiel</i>	Solvent dielectric constant
<i>solventRadius</i>	Solvent probe radius for surfaces that use it (A)
<i>focusFlag</i>	1 if focusing operation, 0 otherwise
<i>sdens</i>	Vacc sphere density
<i>z_mem</i>	Membrane location (A)
<i>L</i>	Membrane thickness (A)
<i>membraneDiel</i>	Membrane dielectric constant
<i>V</i>	Transmembrane potential (V)

Definition at line 246 of file [vpbe.c](#).

7.23.3.2 Vpbe_ctor2()

```

VEXTERNC int Vpbe_ctor2 (
    Vpbe * thee,
    Valist * alist,
    int ionNum,
    double * ionConc,
    double * ionRadii,
    double * ionQ,
    double T,
    double soluteDiel,

```

```

double solventDiel,
double solventRadius,
int focusFlag,
double sdens,
double z_mem,
double L,
double membraneDiel,
double V )

```

FORTRAN stub to construct Vpbe objct.

Author

Nathan Baker and Mike Holst and Michael Grabe

Note

This is partially based on some of Mike Holst's PMG code. Here are a few of the original function comments: kappa is defined as follows:

$$\kappa^2 = \frac{8\pi N_A e_c^2 I_s}{1000 \epsilon_s \epsilon_w k_B T}$$

where the units are esu*esu/erg/mol. To obtain cm^{-2} , we multiply by 10^{-16} . Thus, in cm^{-2} , where k_B and e_c are in gaussian rather than mks units, the proper value for kappa is:

$$\kappa^2 = \frac{8\pi N_A e_c^2 I_s}{1000 \epsilon_s \epsilon_w k_B T} \times 10^{-16}$$

and the factor of 10^{-16} results from converting cm^2 to angstroms^2 , noting that the 1000 in the denominator has converted m^3 to cm^3 , since the ionic strength I_s is assumed to have been provided in moles per liter, which is moles per 1000 cm^3 .

Bug The focusing flag is currently not used!!

Returns

1 if successful, 0 otherwise

Parameters

<i>thee</i>	Pointer to memory allocated for Vpbe object
<i>alist</i>	Atom list
<i>ionNum</i>	Number of counterion species
<i>ionConc</i>	Array containing counterion concentrations (M)
<i>ionRadii</i>	Array containing counterion radii (A)
<i>ionQ</i>	Array containing counterion charges (e)
<i>T</i>	Temperature for Boltzmann distribution (K)
<i>soluteDiel</i>	Solute internal dielectric constant
<i>solventDiel</i>	Solvent dielectric constant
<i>solventRadius</i>	Solvent probe radius for surfaces that use it (A)
<i>focusFlag</i>	1 if focusing operation, 0 otherwise
<i>sdens</i>	Vacc sphere density
<i>z_mem</i>	Membrane location (A)
<i>L</i>	Membrane thickness (A)
<i>membraneDiel</i>	Membrane dielectric constant
<i>V</i>	Transmembrane potential (V)

Definition at line 264 of file [vpbe.c](#).

7.23.3.3 Vpbe_dtor()

```
VEXTERNC void Vpbe_dtor (
    Vpbe ** thee )
```

Object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to memory location of object to be destroyed
-------------	--

Definition at line 467 of file [vpbe.c](#).

7.23.3.4 Vpbe_dtor2()

```
VEXTERNC void Vpbe_dtor2 (
    Vpbe * thee )
```

FORTTRAN stub object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to object to be destroyed
-------------	-----------------------------------

Definition at line 475 of file [vpbe.c](#).

7.23.3.5 Vpbe_getBulkIonicStrength()

```
VEXTERNC double Vpbe_getBulkIonicStrength (
    Vpbe * thee )
```

Get bulk ionic strength.

Author

Nathan Baker

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

Returns

Bulk ionic strength (M)

Definition at line 84 of file [vpbe.c](#).

7.23.3.6 Vpbe_getCoulombEnergy1()

```
VEXTERNC double Vpbe_getCoulombEnergy1 (
    Vpbe * thee )
```

Calculate coulombic energy of set of charges.

Perform an inefficient double sum to calculate the Coulombic energy of a set of charges in a homogeneous dielectric (with

permittivity equal to the protein interior

strength. Result is returned in units of $k_B T$. The sum can be restricted to charges present in simplices of specified color (pcolor); if (color == -1) no restrictions are used.

Author

Nathan Baker

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

Returns

Coulombic energy in units of $k_B T$.

Definition at line 481 of file [vpbe.c](#).

7.23.3.7 Vpbe_getDeblen()

```
VEXTERNC double Vpbe_getDeblen (
    Vpbe * thee )
```

Get Debye-Huckel screening length.

Author

Nathan Baker

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

Returns

Debye-Huckel screening length (Å)

Definition at line 141 of file [vpbe.c](#).

7.23.3.8 Vpbe_getGamma()

```
VEXTERNC double Vpbe_getGamma (
    Vpbe * thee )
```

Get apolar coefficient.

Author

Nathan Baker

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

Returns

Apolar coefficient (kJ/mol/Å²)

7.23.3.9 Vpbe_getIons()

```
VEXTERNC int Vpbe_getIons (
    Vpbe * thee,
    int * nion,
    double ionConc[MAXION],
    double ionRadii[MAXION],
    double ionQ[MAXION] )
```

Get information about the counterion species present.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to Vpbe object
<i>nion</i>	Set to the number of counterion species
<i>ionConc</i>	Array to store counterion species' concentrations (M)
<i>ionRadii</i>	Array to store counterion species' radii (Å)
<i>ionQ</i>	Array to store counterion species' charges (e)

Returns

Number of ions

Definition at line 535 of file [vpbe.c](#).

7.23.3.10 Vpbe_getLmem()

```
VEXTERNC double Vpbe_getLmem (
    Vpbe * thee )
```

Get length of the membrane (Å)

author Michael Grabe.

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

Returns

Length of the membrane (A)

Definition at line 209 of file [vpbe.c](#).

7.23.3.11 Vpbe_getMaxIonRadius()

```
EXTERNC double Vpbe_getMaxIonRadius (
    Vpbe * thee )
```

Get maximum radius of ion species.

Author

Nathan Baker

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

Returns

Maximum radius (A)

Definition at line 127 of file [vpbe.c](#).

7.23.3.12 Vpbe_getmembraneDiel()

```
EXTERNC double Vpbe_getmembraneDiel (
    Vpbe * thee )
```

Get membrane dielectric constant.

Author

Michael Grabe

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

Returns

Membrane dielectric constant

Definition at line 221 of file [vpbe.c](#).

7.23.3.13 Vpbe_getmemv()

```
EXTERNC double Vpbe_getmemv (
    Vpbe * thee )
```

Get membrane potential (kT)

Author

Michael Grabe

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

Definition at line 233 of file [vpbe.c](#).

7.23.3.14 Vpbe_getSoluteCenter()

```
VEXTERNC double * Vpbe_getSoluteCenter (
    Vpbe * thee )
```

Get coordinates of solute center.

Author

Nathan Baker

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

Returns

Pointer to 3*double array with solute center coordinates (A)

Definition at line 107 of file [vpbe.c](#).

7.23.3.15 Vpbe_getSoluteCharge()

```
VEXTERNC double Vpbe_getSoluteCharge (
    Vpbe * thee )
```

Get total solute charge.

Author

Nathan Baker

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

Returns

Total solute charge (e)

Definition at line 186 of file [vpbe.c](#).

7.23.3.16 Vpbe_getSoluteDiel()

```
VEXTERNC double Vpbe_getSoluteDiel (
    Vpbe * thee )
```

Get solute dielectric constant.

Author

Nathan Baker

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

Returns

Solute dielectric constant

Definition at line 99 of file [vpbe.c](#).

7.23.3.17 Vpbe_getSoluteRadius()

```
VEXTERNC double Vpbe_getSoluteRadius (  
    Vpbe * thee )
```

Get sphere radius which bounds biomolecule.

Author

Nathan Baker

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

Returns

Sphere radius which bounds biomolecule (A)

Definition at line 162 of file [vpbe.c](#).

7.23.3.18 Vpbe_getSoluteXlen()

```
VEXTERNC double Vpbe_getSoluteXlen (  
    Vpbe * thee )
```

Get length of solute in x dimension.

Author

Nathan Baker

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

Returns

Length of solute in x dimension (A)

Definition at line 168 of file [vpbe.c](#).

7.23.3.19 Vpbe_getSoluteYlen()

```
VEXTERNC double Vpbe_getSoluteYlen (  
    Vpbe * thee )
```

Get length of solute in y dimension.

Author

Nathan Baker

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

Returns

Length of solute in y dimension (A)

Definition at line 174 of file [vpbe.c](#).**7.23.3.20 Vpbe_getSoluteZlen()**

```
VEXTERNC double Vpbe_getSoluteZlen (
    Vpbe * thee )
```

Get length of solute in z dimension.

Author

Nathan Baker

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

Returns

Length of solute in z dimension (A)

Definition at line 180 of file [vpbe.c](#).**7.23.3.21 Vpbe_getSolventDiel()**

```
VEXTERNC double Vpbe_getSolventDiel (
    Vpbe * thee )
```

Get solvent dielectric constant.

Author

Nathan Baker

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

Returns

Solvent dielectric constant

Definition at line 113 of file [vpbe.c](#).

7.23.3.22 Vpbe_getSolventRadius()

```
VEXTERNC double Vpbe_getSolventRadius (
    Vpbe * thee )
```

Get solvent molecule radius.

Author

Nathan Baker

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

Returns

Solvent molecule radius (A)

Definition at line 120 of file [vpbe.c](#).

7.23.3.23 Vpbe_getTemperature()

```
VEXTERNC double Vpbe_getTemperature (
    Vpbe * thee )
```

Get temperature.

Author

Nathan Baker

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

Returns

Temperature (K)

Definition at line 91 of file [vpbe.c](#).

7.23.3.24 Vpbe_getVacc()

```
VEXTERNC Vacc * Vpbe_getVacc (
    Vpbe * thee )
```

Get accessibility oracle.

Author

Nathan Baker

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

Returns

Pointer to internal Vpbe object

Definition at line 76 of file [vpbe.c](#).

7.23.3.25 Vpbe_getValist()

```
VEXTERNC Valist * Vpbe_getValist (  
    Vpbe * thee )
```

Get atom list.

Author

Nathan Baker

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

Returns

Pointer to internal Valist object

Definition at line 69 of file [vpbe.c](#).

7.23.3.26 Vpbe_getXkappa()

```
VEXTERNC double Vpbe_getXkappa (  
    Vpbe * thee )
```

Get Debye-Huckel parameter.

Author

Nathan Baker

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

Returns

Bulk Debye-Huckel parameter (Å)

Definition at line 134 of file [vpbe.c](#).

7.23.3.27 Vpbe_getZkappa2()

```
VEXTERNC double Vpbe_getZkappa2 (  
    Vpbe * thee )
```

Get modified squared Debye-Huckel parameter.

Author

Nathan Baker

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

Returns

Modified squared Debye-Huckel parameter (^{-2})

Definition at line 148 of file [vpbe.c](#).

7.23.3.28 Vpbe_getZmagic()

```
VEXTERNC double Vpbe_getZmagic (  
    Vpbe * thee )
```

Get charge scaling factor.

Author

Nathan Baker and Mike Holst

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

Returns

Get factor for scaling charges (in e) to internal units

Definition at line 155 of file [vpbe.c](#).

7.23.3.29 Vpbe_getzmem()

```
VEXTERNC double Vpbe_getzmem (  
    Vpbe * thee )
```

Get z position of the membrane bottom.

Author

Michael Grabe

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

Returns

z value of membrane (A)

Definition at line 197 of file [vpbe.c](#).

7.23.3.30 Vpbe_memChk()

```

VEXTERNC unsigned long int Vpbe_memChk (
    Vpbe * thee )

```

Return the memory used by this structure (and its contents) in bytes.

Author

Nathan Baker

Parameters

<i>thee</i>	Vpbe object
-------------	-------------

Returns

The memory used by this structure and its contents in bytes

Definition at line 523 of file [vpbe.c](#).

7.24 Vstring class

Provides a collection of useful non-ANSI string functions.

Files

- file [vstring.c](#)
Class Vstring methods.
- file [vstring.h](#)
Contains declarations for class Vstring.

Functions

- char * [Vstring_wrappedtext](#) (const char *str, int right_margin, int left_padding)
- VEXTERNC int [Vstring_strcasecmp](#) (const char *s1, const char *s2)
Case-insensitive string comparison (BSD standard)
- VEXTERNC int [Vstring_isdigit](#) (const char *tok)
A modified sscanf that examines the complete string.

7.24.1 Detailed Description

Provides a collection of useful non-ANSI string functions.

7.24.2 Function Documentation

7.24.2.1 Vstring_isdigit()

```

VEXTERNC int Vstring_isdigit (
    const char * tok )

```

A modified sscanf that examines the complete string.

Author

Todd Dolinsky

Parameters

<i>tok</i>	The string to examine
------------	-----------------------

Returns

1 if the entire string is an integer, 0 if otherwise.

Definition at line 130 of file [vstring.c](#).

7.24.2.2 Vstring_strcasecmp()

```
EXTERNC int Vstring_strcasecmp (  
    const char * s1,  
    const char * s2 )
```

Case-insensitive string comparison (BSD standard)

Author

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Note

Copyright (c) 1988-1993 The Regents of the University of California. Copyright (c) 1995-1996 Sun Microsystems, Inc.

Parameters

<i>s1</i>	First string for comparison
<i>s2</i>	Second string for comparison

Returns

An integer less than, equal to, or greater than zero if s1 is found, respectively, to be less than, to match, or be greater than s2. (Source: Linux man pages)

Definition at line 66 of file [vstring.c](#).

7.24.2.3 Vstring_wrappedtext()

```
EXTERNC char * Vstring_wrappedtext (  
    const char * str,  
    int right_margin,  
    int left_padding )
```

Creates a wrapped and indented string from an input string

Author

Tucker Beck

Note

This function allocates a new string, so be sure to free it!

Creates a wrapped and indented string from an input string

Author

Tucker Beck

Note

This function allocates a new string, so be sure to free it!

Note

: The +2 is for the newline character and the null-terminating character;

Parameters

<i>str</i>	The input string to wrap and indent
<i>right_margin</i>	The number of characters to the right margin
<i>left_padding</i>	The number of characters in the left indent

Definition at line 155 of file [vstring.c](#).

7.25 Vunit class

Collection of constants and conversion factors.

Files

- file [vunit.h](#)
Contains a collection of useful constants and conversion factors.

Macros

- #define [Vunit_J_to_cal](#) 4.1840000e+00
Multiply by this to convert J to cal.
- #define [Vunit_cal_to_J](#) 2.3900574e-01
Multiply by this to convert cal to J.
- #define [Vunit_amu_to_kg](#) 1.6605402e-27
Multiply by this to convert amu to kg.
- #define [Vunit_kg_to_amu](#) 6.0221367e+26
Multiply by this to convert kg to amu.
- #define [Vunit_ec_to_C](#) 1.6021773e-19
Multiply by this to convert ec to C.
- #define [Vunit_C_to_ec](#) 6.2415065e+18
Multiply by this to convert C to ec.
- #define [Vunit_ec](#) 1.6021773e-19
Charge of an electron in C.
- #define [Vunit_kb](#) 1.3806581e-23

- *Boltzmann constant.*
• #define `Vunit_Na` 6.0221367e+23
- *Avogadro's number.*
• #define `Vunit_pi` VPI
- *Pi.*
• #define `Vunit_eps0` 8.8541878e-12
- *Vacuum permittivity.*
• #define `Vunit_esu_ec2A` 3.3206364e+02
- *e_c^2 / in ESU units => kcal/mol*
• #define `Vunit_esu_kb` 1.9871913e-03
- *k_b in ESU units => kcal/mol*

7.25.1 Detailed Description

Collection of constants and conversion factors.

7.25.2 Macro Definition Documentation

7.25.2.1 Vunit_amu_to_kg

```
#define Vunit_amu_to_kg 1.6605402e-27
```

Multiply by this to convert amu to kg.

Definition at line 76 of file [vunit.h](#).

7.25.2.2 Vunit_C_to_ec

```
#define Vunit_C_to_ec 6.2415065e+18
```

Multiply by this to convert C to ec.

Definition at line 88 of file [vunit.h](#).

7.25.2.3 Vunit_cal_to_J

```
#define Vunit_cal_to_J 2.3900574e-01
```

Multiply by this to convert cal to J.

Definition at line 72 of file [vunit.h](#).

7.25.2.4 Vunit_ec

```
#define Vunit_ec 1.6021773e-19
```

Charge of an electron in C.

Definition at line 92 of file [vunit.h](#).

7.25.2.5 Vunit_ec_to_C

```
#define Vunit_ec_to_C 1.6021773e-19
```

Multiply by this to convert ec to C.

Definition at line 84 of file [vunit.h](#).

7.25.2.6 Vunit_eps0

```
#define Vunit_eps0 8.8541878e-12
```

Vacuum permittivity.

Definition at line 108 of file [vunit.h](#).

7.25.2.7 Vunit_esu_ec2A

```
#define Vunit_esu_ec2A 3.3206364e+02
```

e_c^2 / in ESU units => kcal/mol
Definition at line 112 of file [vunit.h](#).

7.25.2.8 Vunit_esu_kb

```
#define Vunit_esu_kb 1.9871913e-03
```

k_b in ESU units => kcal/mol
Definition at line 116 of file [vunit.h](#).

7.25.2.9 Vunit_J_to_cal

```
#define Vunit_J_to_cal 4.1840000e+00
```

Multiply by this to convert J to cal.
Definition at line 68 of file [vunit.h](#).

7.25.2.10 Vunit_kb

```
#define Vunit_kb 1.3806581e-23
```

Boltzmann constant.
Definition at line 96 of file [vunit.h](#).

7.25.2.11 Vunit_kg_to_amu

```
#define Vunit_kg_to_amu 6.0221367e+26
```

Multiply by this to convert kg to amu.
Definition at line 80 of file [vunit.h](#).

7.25.2.12 Vunit_Na

```
#define Vunit_Na 6.0221367e+23
```

Avogadro's number.
Definition at line 100 of file [vunit.h](#).

7.25.2.13 Vunit_pi

```
#define Vunit_pi VPI
```

Pi.
Definition at line 104 of file [vunit.h](#).

7.26 Vgrid class

Oracle for Cartesian mesh data.

Files

- file [vgrid.c](#)
Class Vgrid methods.
- file [vgrid.h](#)
Potential oracle for Cartesian mesh data.

Data Structures

- struct [sVgrid](#)

Electrostatic potential oracle for Cartesian mesh data.

Macros

- #define [VGRID_DIGITS](#) 6

Number of decimal places for comparisons and formatting.

Typedefs

- typedef struct [sVgrid](#) [Vgrid](#)

Declaration of the Vgrid class as the [sVgrid](#) structure.

Functions

- VEXTERNC unsigned long int [Vgrid_memChk](#) ([Vgrid](#) *thee)
Return the memory used by this structure (and its contents) in bytes.
- VEXTERNC [Vgrid](#) * [Vgrid_ctor](#) (int nx, int ny, int nz, double hx, double hy, double hzed, double xmin, double ymin, double zmin, double *data)
Construct Vgrid object with values obtained from Vpmg_readDX (for example)
- VEXTERNC int [Vgrid_ctor2](#) ([Vgrid](#) *thee, int nx, int ny, int nz, double hx, double hy, double hzed, double xmin, double ymin, double zmin, double *data)
Initialize Vgrid object with values obtained from Vpmg_readDX (for example)
- VEXTERNC int [Vgrid_value](#) ([Vgrid](#) *thee, double x[3], double *value)
Get potential value (from mesh or approximation) at a point.
- VEXTERNC void [Vgrid_dtor](#) ([Vgrid](#) **thee)
Object destructor.
- VEXTERNC void [Vgrid_dtor2](#) ([Vgrid](#) *thee)
FORTTRAN stub object destructor.
- VEXTERNC int [Vgrid_curvature](#) ([Vgrid](#) *thee, double pt[3], int cflag, double *curv)
Get second derivative values at a point.
- VEXTERNC int [Vgrid_gradient](#) ([Vgrid](#) *thee, double pt[3], double grad[3])
Get first derivative values at a point.
- VEXTERNC int [Vgrid_readGZ](#) ([Vgrid](#) *thee, const char *fname)
Read in OpenDX data in GZIP format.
- VEXTERNC void [Vgrid_writeUHBD](#) ([Vgrid](#) *thee, const char *iodev, const char *iofmt, const char *thost, const char *fname, char *title, double *pvec)
Write out the data in UHBD grid format.
- VEXTERNC void [Vgrid_writeDX](#) ([Vgrid](#) *thee, const char *iodev, const char *iofmt, const char *thost, const char *fname, char *title, double *pvec)
Write out the data in OpenDX grid format.
- VEXTERNC int [Vgrid_readDX](#) ([Vgrid](#) *thee, const char *iodev, const char *iofmt, const char *thost, const char *fname)
Read in data in OpenDX grid format.
- VEXTERNC void [Vgrid_writeDXBIN](#) ([Vgrid](#) *thee, const char *iodev, const char *iofmt, const char *thost, const char *fname, char *title, double *pvec)
Write out the binary data in OpenDX grid format.

- VEXTERNC int `Vgrid_readDXBIN` (`Vgrid *thee`, const char *iodev, const char *iofmt, const char *thost, const char *fname)
Read in binary data in OpenDX grid format.
- VEXTERNC double `Vgrid_integrate` (`Vgrid *thee`)
Get the integral of the data.
- VEXTERNC double `Vgrid_normL1` (`Vgrid *thee`)
Get the L_1 norm of the data. This returns the integral:
- VEXTERNC double `Vgrid_normL2` (`Vgrid *thee`)
Get the L_2 norm of the data. This returns the integral:
- VEXTERNC double `Vgrid_normLinf` (`Vgrid *thee`)
Get the L_∞ norm of the data. This returns the integral:
- VEXTERNC double `Vgrid_seminormH1` (`Vgrid *thee`)
Get the H_1 semi-norm of the data. This returns the integral:
- VEXTERNC double `Vgrid_normH1` (`Vgrid *thee`)
Get the H_1 norm (or energy norm) of the data. This returns the integral:

7.26.1 Detailed Description

Oracle for Cartesian mesh data.

7.26.2 Macro Definition Documentation

7.26.2.1 VGRID_DIGITS

```
#define VGRID_DIGITS 6
```

Number of decimal places for comparisons and formatting.

Definition at line 74 of file [vgrid.h](#).

7.26.3 Typedef Documentation

7.26.3.1 Vgrid

```
typedef struct sVgrid Vgrid
```

Declaration of the Vgrid class as the `sVgrid` structure.

Definition at line 106 of file [vgrid.h](#).

7.26.4 Function Documentation

7.26.4.1 Vgrid_ctor()

```
VEXTERNC Vgrid * Vgrid_ctor (
    int nx,
    int ny,
    int nz,
    double hx,
    double hy,
    double hzed,
    double xmin,
    double ymin,
    double zmin,
    double * data )
```

Construct Vgrid object with values obtained from `Vpmg_readDX` (for example)

Author

Nathan Baker

Parameters

<i>nx</i>	Number grid points in x direction
<i>ny</i>	Number grid points in y direction
<i>nz</i>	Number grid points in z direction
<i>hx</i>	Grid spacing in x direction
<i>hy</i>	Grid spacing in y direction
<i>hz</i>	Grid spacing in z direction
<i>xmin</i>	x coordinate of lower grid corner
<i>ymin</i>	y coordinate of lower grid corner
<i>zmin</i>	z coordinate of lower grid corner
<i>data</i>	nx*ny*nz array of data. This can be VNULL if you are planning to read in data later with one of the read routines

Returns

Newly allocated and initialized Vgrid object

Definition at line 86 of file [vgrid.c](#).**7.26.4.2 Vgrid_ctor2()**

```

VEXTERNC int Vgrid_ctor2 (
    Vgrid * thee,
    int nx,
    int ny,
    int nz,
    double hx,
    double hy,
    double hz,
    double xmin,
    double ymin,
    double zmin,
    double * data )

```

Initialize Vgrid object with values obtained from Vpmg_readDX (for example)

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to newly allocated Vgrid object
<i>nx</i>	Number grid points in x direction
<i>ny</i>	Number grid points in y direction
<i>nz</i>	Number grid points in z direction
<i>hx</i>	Grid spacing in x direction
<i>hy</i>	Grid spacing in y direction

Parameters

<i>hzed</i>	Grid spacing in z direction
<i>xmin</i>	x coordinate of lower grid corner
<i>ymin</i>	y coordinate of lower grid corner
<i>zmin</i>	z coordinate of lower grid corner
<i>data</i>	nx*ny*nz array of data. This can be VNULL if you are planning to read in data later with one of the read routines

Returns

Newly allocated and initialized Vgrid object

Definition at line 112 of file [vgrid.c](#).

7.26.4.3 Vgrid_curvature()

```

VEXTERNC int Vgrid_curvature (
    Vgrid * thee,
    double pt[3],
    int cflag,
    double * curv )

```

Get second derivative values at a point.

Author

Steve Bond and Nathan Baker

Parameters

<i>thee</i>	Pointer to Vgrid object
<i>pt</i>	Location to evaluate second derivative
<i>cflag</i>	<ul style="list-style-type: none"> • 0: Reduced Maximal Curvature • 1: Mean Curvature (Laplace) • 2: Gauss Curvature • 3: True Maximal Curvature
<i>curv</i>	Specified curvature value

Returns

1 if successful, 0 if off grid

Definition at line 299 of file [vgrid.c](#).

7.26.4.4 Vgrid_dtor()

```

VEXTERNC void Vgrid_dtor (
    Vgrid ** thee )

```

Object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to memory location of object to be destroyed
-------------	--

Definition at line 152 of file [vgrid.c](#).**7.26.4.5 Vgrid_dtor2()**

```
VEXTERNC void Vgrid_dtor2 (
    Vgrid * thee )
```

FORTRAN stub object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to object to be destroyed
-------------	-----------------------------------

Definition at line 165 of file [vgrid.c](#).**7.26.4.6 Vgrid_gradient()**

```
VEXTERNC int Vgrid_gradient (
    Vgrid * thee,
    double pt[3],
    double grad[3] )
```

Get first derivative values at a point.

Author

Nathan Baker and Steve Bond

Parameters

<i>thee</i>	Pointer to Vgrid object
<i>pt</i>	Location to evaluate gradient
<i>grad</i>	Gradient

Returns

1 if successful, 0 if off grid

Definition at line 379 of file [vgrid.c](#).**7.26.4.7 Vgrid_integrate()**

```
VEXTERNC double Vgrid_integrate (
    Vgrid * thee )
```

Get the integral of the data.

Author

Nathan Baker

Parameters

<i>thee</i>	Vgrid object
-------------	--------------

Returns

Integral of data

Definition at line 1790 of file [vgrid.c](#).**7.26.4.8 Vgrid_memChk()**

```

VEXTERNC unsigned long int Vgrid_memChk (
    Vgrid * thee )

```

Return the memory used by this structure (and its contents) in bytes.

Author

Nathan Baker

Parameters

<i>thee</i>	Vgrid object
-------------	--------------

Returns

The memory used by this structure and its contents in bytes

Definition at line 63 of file [vgrid.c](#).**7.26.4.9 Vgrid_normH1()**

```

VEXTERNC double Vgrid_normH1 (
    Vgrid * thee )

```

Get the H_1 norm (or energy norm) of the data. This returns the integral:**Author**

Nathan Baker

Parameters

<i>thee</i>	Vgrid object
-------------	--------------

Returns

Integral of data

$$\|u\|_{H_1} = \left(\int_{\Omega} |\nabla u(x)|^2 dx + \int_{\Omega} |u(x)|^2 dx \right)^{1/2}$$

Definition at line 1931 of file [vgrid.c](#).

7.26.4.10 Vgrid_normL1()

```
VEXTERNC double Vgrid_normL1 (
    Vgrid * thee )
```

Get the L_1 norm of the data. This returns the integral:

Author

Nathan Baker

Parameters

<i>thee</i>	Vgrid object
-------------	--------------

Returns

L_1 norm of data

$$\|u\|_{L_1} = \int_{\Omega} |u(x)| dx$$

Definition at line 1828 of file [vgrid.c](#).

7.26.4.11 Vgrid_normL2()

```
VEXTERNC double Vgrid_normL2 (
    Vgrid * thee )
```

Get the L_2 norm of the data. This returns the integral:

Author

Nathan Baker

Parameters

<i>thee</i>	Vgrid object
-------------	--------------

Returns

L_2 norm of data

$$\|u\|_{L_2} = \left(\int_{\Omega} |u(x)|^2 dx \right)^{1/2}$$

Definition at line 1858 of file [vgrid.c](#).

7.26.4.12 Vgrid_normLinf()

```
VEXTERNC double Vgrid_normLinf (
    Vgrid * thee )
```

Get the L_{∞} norm of the data. This returns the integral:

Author

Nathan Baker

Parameters

<i>thee</i>	Vgrid object
-------------	--------------

Returns

L_∞ norm of data

$$\|u\|_{L_\infty} = \sup_{x \in \Omega} |u(x)|$$

Definition at line 1946 of file [vgrid.c](#).

7.26.4.13 Vgrid_readDX()

```
VEXTERNC int Vgrid_readDX (
    Vgrid * thee,
    const char * iodev,
    const char * iofmt,
    const char * thost,
    const char * fname )
```

Read in data in OpenDX grid format.

Note

All dimension information is given in order: z, y, x

Author

Nathan Baker

Parameters

<i>thee</i>	Vgrid object
<i>iodev</i>	Input device type (FILE/BUFF/UNIX/INET)
<i>iofmt</i>	Input device format (ASCII/XDR)
<i>thost</i>	Input hostname (for sockets)
<i>fname</i>	Input FILE/BUFF/UNIX/INET name

Returns

1 if successful, 0 otherwise

Load grid from an input file using sockets.

Author

Nathan Baker

Definition at line 586 of file [vgrid.c](#).

7.26.4.14 Vgrid_readDXBIN()

```
VEXTERNC int Vgrid_readDXBIN (
    Vgrid * thee,
    const char * iodev,
    const char * iofmt,
```

```
const char * thost,
const char * fname )
```

Read in binary data in OpenDX grid format.

Note

All dimension information is given in order: z, y, x

Author

Juan Brandi

Parameters

<i>thee</i>	Vgrid object
<i>iodev</i>	Input device type (FILE/BUFF/UNIX/INET)
<i>iofmt</i>	Input device format (ASCII/XDR)
<i>thost</i>	Input hostname (for sockets)
<i>fname</i>	Input FILE/BUFF/UNIX/INET name

Returns

1 if successful, 0 otherwise

Load grid from an input dx binary file.

Author

Juan Brandi

Definition at line [810](#) of file [vgrid.c](#).

7.26.4.15 Vgrid_readGZ()

```
VEXTERNC int Vgrid_readGZ (
    Vgrid * thee,
    const char * fname )
```

Read in OpenDX data in GZIP format.

Author

Dave Gohara

Returns

1 if successful, 0 otherwise

Parameters

<i>thee</i>	Object with grid data to write
<i>fname</i>	Path to write to

Definition at line [462](#) of file [vgrid.c](#).

7.26.4.16 Vgrid_seminormH1()

```
VEXTERNC double Vgrid_seminormH1 (
    Vgrid * thee )
```

Get the H_1 semi-norm of the data. This returns the integral:

Author

Nathan Baker

Parameters

<i>thee</i>	Vgrid object
-------------	--------------

Returns

Integral of data

$$|u|_{H_1} = \left(\int_{\Omega} |\nabla u(x)|^2 dx \right)^{1/2}$$

Definition at line 1888 of file [vgrid.c](#).

7.26.4.17 Vgrid_value()

```
VEXTERNC int Vgrid_value (
    Vgrid * thee,
    double x[3],
    double * value )
```

Get potential value (from mesh or approximation) at a point.

Author

Nathan Baker

Parameters

<i>thee</i>	Vgrid object
<i>x</i>	Point at which to evaluate potential
<i>value</i>	Value of data at point x

Returns

1 if successful, 0 if off grid

Definition at line 179 of file [vgrid.c](#).

7.26.4.18 Vgrid_writeDX()

```
VEXTERNC void Vgrid_writeDX (
    Vgrid * thee,
    const char * iodev,
    const char * iofmt,
    const char * thost,
    const char * fname,
```

```
char * title,
double * pvec )
```

Write out the data in OpenDX grid format.

Author

Nathan Baker

Parameters

<i>thee</i>	Grid object
<i>iodev</i>	Output device type (FILE/BUFF/UNIX/INET)
<i>iofmt</i>	Output device format (ASCII/XDR)
<i>thost</i>	Output hostname (for sockets)
<i>fname</i>	Output FILE/BUFF/UNIX/INET name
<i>title</i>	Title to be inserted in grid file
<i>pvec</i>	Partition weight (if 1: point in current partition, if 0 point not in current partition if > 0 && < 1 point on/near boundary)

Definition at line 1206 of file [vgrid.c](#).

7.26.4.19 Vgrid_writeDXBIN()

```
VEXTERNC void Vgrid_writeDXBIN (
    Vgrid * thee,
    const char * iodev,
    const char * iofmt,
    const char * thost,
    const char * fname,
    char * title,
    double * pvec )
```

Write out the binary data in OpenDX grid format.

Author

Nathan Baker

Parameters

<i>thee</i>	Grid object
<i>iodev</i>	Output device type (FILE/BUFF/UNIX/INET)
<i>iofmt</i>	Output device format (ASCII/XDR)
<i>thost</i>	Output hostname (for sockets)
<i>fname</i>	Output FILE/BUFF/UNIX/INET name
<i>title</i>	Title to be inserted in grid file
<i>pvec</i>	Partition weight (if 1: point in current partition, if 0 point not in current partition if > 0 && < 1 point on/near boundary)

Definition at line 1458 of file [vgrid.c](#).

7.26.4.20 Vgrid_writeUHBD()

```

VEXTERNC void Vgrid_writeUHBD (
    Vgrid * thee,
    const char * iodev,
    const char * iofmt,
    const char * thost,
    const char * fname,
    char * title,
    double * pvec )

```

Write out the data in UHBD grid format.

Note

- The mesh spacing should be uniform
- Format changed from %12.6E to %12.5E

Author

Nathan Baker

Parameters

<i>thee</i>	Grid object
<i>iodev</i>	Output device type (FILE/BUFF/UNIX/INET)
<i>iofmt</i>	Output device format (ASCII/XDR)
<i>thost</i>	Output hostname (for sockets)
<i>fname</i>	Output FILE/BUFF/UNIX/INET name
<i>title</i>	Title to be inserted in grid file
<i>pvec</i>	Partition weight (if 1: point in current partition, if 0 point not in current partition if > 0 && < 1 point on/near boundary)

Bug This routine does not respect partition information

Definition at line 1692 of file [vgrid.c](#).

7.27 Vmgrid class

Oracle for Cartesian mesh data.

Files

- file [vmgrid.c](#)
Class Vmgrid methods.
- file [vmgrid.h](#)
Multiresolution oracle for Cartesian mesh data.

Data Structures

- struct [sVmgrid](#)
Multiresolution oracle for Cartesian mesh data.

Macros

- `#define VMGRIDMAX 20`
The maximum number of levels in the grid hierarchy.

Typedefs

- `typedef struct sVmgrid Vmgrid`
Declaration of the Vmgrid class as the Vmgrid structure.

Functions

- `VEXTERNC Vmgrid * Vmgrid_ctor ()`
Construct Vmgrid object.
- `VEXTERNC int Vmgrid_ctor2 (Vmgrid *thee)`
Initialize Vmgrid object.
- `VEXTERNC int Vmgrid_value (Vmgrid *thee, double x[3], double *value)`
Get potential value (from mesh or approximation) at a point.
- `VEXTERNC void Vmgrid_dtor (Vmgrid **thee)`
Object destructor.
- `VEXTERNC void Vmgrid_dtor2 (Vmgrid *thee)`
FORTTRAN stub object destructor.
- `VEXTERNC int Vmgrid_addGrid (Vmgrid *thee, Vgrid *grid)`
Add a grid to the hierarchy.
- `VEXTERNC int Vmgrid_curvature (Vmgrid *thee, double pt[3], int cflag, double *curv)`
Get second derivative values at a point.
- `VEXTERNC int Vmgrid_gradient (Vmgrid *thee, double pt[3], double grad[3])`
Get first derivative values at a point.
- `VEXTERNC Vgrid * Vmgrid_getGridByNum (Vmgrid *thee, int num)`
Get specific grid in hierarchy.
- `VEXTERNC Vgrid * Vmgrid_getGridByPoint (Vmgrid *thee, double pt[3])`
Get grid in hierarchy which contains specified point or VNULL.

7.27.1 Detailed Description

Oracle for Cartesian mesh data.

7.27.2 Macro Definition Documentation

7.27.2.1 VMGRIDMAX

```
#define VMGRIDMAX 20
```

The maximum number of levels in the grid hierarchy.

Definition at line 76 of file [vmgrid.h](#).

7.27.3 Typedef Documentation

7.27.3.1 Vmgrid

```
typedef struct sVmgrid Vmgrid
```

Declaration of the Vmgrid class as the Vmgrid structure.

Definition at line 98 of file [vmgrid.h](#).

7.27.4 Function Documentation

7.27.4.1 Vmgrid_addGrid()

```
VEXTERNC int Vmgrid_addGrid (
    Vmgrid * thee,
    Vgrid * grid )
```

Add a grid to the hierarchy.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to object to be destroyed
<i>grid</i>	Grid to be added. As mentioned above, we would prefer to have the finest grid added first, next-finest second, ..., coarsest last – this is how the grid will be searched when looking up values for points. However, this is not enforced to provide flexibility for cases where the dataset is decomposed into disjoint partitions, etc.

Returns

1 if successful, 0 otherwise

Definition at line 195 of file [vmgrid.c](#).

7.27.4.2 Vmgrid_ctor()

```
VEXTERNC Vmgrid * Vmgrid_ctor ( )
```

Construct Vmgrid object.

Author

Nathan Baker

Returns

Newly allocated and initialized Vmgrid object

Definition at line 57 of file [vmgrid.c](#).

7.27.4.3 Vmgrid_ctor2()

```
VEXTERNC int Vmgrid_ctor2 (
    Vmgrid * thee )
```

Initialize Vmgrid object.

Author

Nathan Baker

Parameters

<i>thee</i>	Newly allocated Vmgrid object
-------------	-------------------------------

Returns

Newly allocated and initialized Vmgrid object

Definition at line 72 of file [vmgrid.c](#).

7.27.4.4 Vmgrid_curvature()

```
VEXTERNC int Vmgrid_curvature (  
    Vmgrid * thee,  
    double pt[3],  
    int cflag,  
    double * curv )
```

Get second derivative values at a point.

Author

Nathan Baker (wrapper for Vgrid routine by Steve Bond)

Parameters

<i>thee</i>	Pointer to Vmgrid object
<i>pt</i>	Location to evaluate second derivative
<i>cflag</i>	<ul style="list-style-type: none">• 0: Reduced Maximal Curvature• 1: Mean Curvature (Laplace)• 2: Gauss Curvature• 3: True Maximal Curvature
<i>curv</i>	Specified curvature value

Returns

1 if successful, 0 if off grid

Definition at line 138 of file [vmgrid.c](#).

7.27.4.5 Vmgrid_dtor()

```
VEXTERNC void Vmgrid_dtor (  
    Vmgrid ** thee )
```

Object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to memory location of object to be destroyed
-------------	--

Definition at line 88 of file [vmgrid.c](#).

7.27.4.6 Vmgrid_dtor2()

```
VEEXTERNAL void Vmgrid_dtor2 (
    Vmgrid * thee )
```

FORTTRAN stub object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to object to be destroyed
-------------	-----------------------------------

Definition at line 101 of file [vmgrid.c](#).

7.27.4.7 Vmgrid_getGridByNum()

```
VEEXTERNAL Vgrid * Vmgrid_getGridByNum (
    Vmgrid * thee,
    int num )
```

Get specific grid in hierarchy.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to Vmgrid object
<i>num</i>	Number of grid in hierarchy

Returns

Pointer to specified grid

7.27.4.8 Vmgrid_getGridByPoint()

```
VEEXTERNAL Vgrid * Vmgrid_getGridByPoint (
    Vmgrid * thee,
    double pt[3] )
```

Get grid in hierarchy which contains specified point or VNULL.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to Vmgrid object
<i>pt</i>	Point to check

Returns

Pointer to specified grid

7.27.4.9 Vmgrid_gradient()

```
VEXTERNC int Vmgrid_gradient (
    Vmgrid * thee,
    double pt[3],
    double grad[3] )
```

Get first derivative values at a point.

Author

Nathan Baker and Steve Bond

Parameters

<i>thee</i>	Pointer to Vmgrid object
<i>pt</i>	Location to evaluate gradient
<i>grad</i>	Gradient

Returns

1 if successful, 0 if off grid

Definition at line 167 of file [vmgrid.c](#).

7.27.4.10 Vmgrid_value()

```
VEXTERNC int Vmgrid_value (
    Vmgrid * thee,
    double x[3],
    double * value )
```

Get potential value (from mesh or approximation) at a point.

Author

Nathan Baker

Parameters

<i>thee</i>	Vmgrid obejct
<i>x</i>	Point at which to evaluate potential
<i>value</i>	Value of data at point x

Returns

1 if successful, 0 if off grid

Definition at line 107 of file [vmgrid.c](#).

7.28 Vopot class

Potential oracle for Cartesian mesh data.

Files

- file [vopot.c](#)
Class Vopot methods.
- file [vopot.h](#)
Potential oracle for Cartesian mesh data.

Data Structures

- struct [sVopot](#)
Electrostatic potential oracle for Cartesian mesh data.

Typedefs

- typedef struct [sVopot](#) [Vopot](#)
Declaration of the Vopot class as the Vopot structure.

Functions

- VEXTERNC [Vopot](#) * [Vopot_ctor](#) ([Vmgrid](#) *mgrid, [Vpbe](#) *pbe, [Vbcfl](#) bcfl)
Construct Vopot object with values obtained from Vpmg_readDX (for example)
- VEXTERNC int [Vopot_ctor2](#) ([Vopot](#) *thee, [Vmgrid](#) *mgrid, [Vpbe](#) *pbe, [Vbcfl](#) bcfl)
Initialize Vopot object with values obtained from Vpmg_readDX (for example)
- VEXTERNC int [Vopot_pot](#) ([Vopot](#) *thee, double x[3], double *pot)
Get potential value (from mesh or approximation) at a point.
- VEXTERNC void [Vopot_dtor](#) ([Vopot](#) **thee)
Object destructor.
- VEXTERNC void [Vopot_dtor2](#) ([Vopot](#) *thee)
FORTTRAN stub object destructor.
- VEXTERNC int [Vopot_curvature](#) ([Vopot](#) *thee, double pt[3], int cflag, double *curv)
Get second derivative values at a point.
- VEXTERNC int [Vopot_gradient](#) ([Vopot](#) *thee, double pt[3], double grad[3])
Get first derivative values at a point.

7.28.1 Detailed Description

Potential oracle for Cartesian mesh data.

7.28.2 Typedef Documentation

7.28.2.1 Vopot

`typedef struct sVopot Vopot`

Declaration of the Vopot class as the Vopot structure.

Definition at line 96 of file [vopot.h](#).

7.28.3 Function Documentation

7.28.3.1 Vopot_ctor()

```
VEXTERNC Vopot * Vopot_ctor (
    Vmgrid * mgrid,
    Vpbe * pbe,
    Vbcfl bcfl )
```

Construct Vopot object with values obtained from Vpmg_readDX (for example)

Author

Nathan Baker

Parameters

<i>mgrid</i>	Multiple grid object containing potential data (in units kT/e)
<i>pbe</i>	Pointer to Vpbe object for parameters
<i>bcfl</i>	Boundary condition to use for potential values off the grid

Returns

Newly allocated and initialized Vopot object

Definition at line 65 of file [vopot.c](#).

7.28.3.2 Vopot_ctor2()

```
VEXTERNC int Vopot_ctor2 (
    Vopot * thee,
    Vmgrid * mgrid,
    Vpbe * pbe,
    Vbcfl bcfl )
```

Initialize Vopot object with values obtained from Vpmg_readDX (for example)

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to newly allocated Vopot object
<i>mgrid</i>	Multiple grid object containing potential data (in units kT/e)
<i>pbe</i>	Pointer to Vpbe object for parameters
<i>bcfl</i>	Boundary condition to use for potential values off the grid

Returns

1 if successful, 0 otherwise

Definition at line 80 of file [vopot.c](#).

7.28.3.3 Vopot_curvature()

```
VEXTERNC int Vopot_curvature (
    Vopot * thee,
    double pt[3],
    int cflag,
    double * curv )
```

Get second derivative values at a point.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to Vopot object
<i>pt</i>	Location to evaluate second derivative
<i>cflag</i>	<ul style="list-style-type: none">• 0: Reduced Maximal Curvature• 1: Mean Curvature (Laplace)• 2: Gauss Curvature• 3: True Maximal Curvature
<i>curv</i>	Set to specified curvature value

Returns

1 if successful, 0 otherwise

Definition at line 214 of file [vopot.c](#).

7.28.3.4 Vopot_dtor()

```
VEXTERNC void Vopot_dtor (
    Vopot ** thee )
```

Object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to memory location of object to be destroyed
-------------	--

Definition at line 94 of file [vopot.c](#).

7.28.3.5 Vopot_dtor2()

```
VEXTERNC void Vopot_dtor2 (
    Vopot * thee )
```

FORTTRAN stub object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to object to be destroyed
-------------	-----------------------------------

Definition at line 107 of file [vopot.c](#).

7.28.3.6 Vopot_gradient()

```
VEXTERNC int Vopot_gradient (
    Vopot * thee,
    double pt[3],
    double grad[3] )
```

Get first derivative values at a point.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to Vopot object
<i>pt</i>	Location to evaluate gradient
<i>grad</i>	Gradient

Returns

1 if successful, 0 otherwise

Definition at line 300 of file [vopot.c](#).

7.28.3.7 Vopot_pot()

```
VEXTERNC int Vopot_pot (
    Vopot * thee,
    double x[3],
    double * pot )
```

Get potential value (from mesh or approximation) at a point.

Author

Nathan Baker

Parameters

<i>thee</i>	Vopot obejct
<i>x</i>	Point at which to evaluate potential
<i>pot</i>	Set to dimensionless potential (units kT/e) at point x

Returns

1 if successful, 0 otherwise

Definition at line 114 of file [vopot.c](#).

7.29 Vpmg class

A wrapper for Mike Holst's PMG multigrid code.

Files

- file [vpmg.c](#)
Class Vpmg methods.
- file [vpmg.h](#)
Contains declarations for class Vpmg.

Data Structures

- struct [sVpmg](#)
Contains public data members for Vpmg class/module.

Typedefs

- typedef struct [sVpmg](#) [Vpmg](#)
Declaration of the Vpmg class as the Vpmg structure.

Functions

- VEXTERNNC unsigned long int [Vpmg_memChk](#) ([Vpmg](#) *thee)
Return the memory used by this structure (and its contents) in bytes.
- VEXTERNNC [Vpmg](#) * [Vpmg_ctor](#) ([Vpmgp](#) *parms, [Vpbe](#) *pbe, int focusFlag, [Vpmg](#) *pmgOLD, [MGparm](#) *mgparm, [PBEparm_calcEnergy](#) energyFlag)
Constructor for the Vpmg class (allocates new memory)
- VEXTERNNC int [Vpmg_ctor2](#) ([Vpmg](#) *thee, [Vpmgp](#) *parms, [Vpbe](#) *pbe, int focusFlag, [Vpmg](#) *pmgOLD, [MGparm](#) *mgparm, [PBEparm_calcEnergy](#) energyFlag)
FORTRAN stub constructor for the Vpmg class (uses previously-allocated memory)
- VEXTERNNC void [Vpmg_dtor](#) ([Vpmg](#) **thee)
Object destructor.
- VEXTERNNC void [Vpmg_dtor2](#) ([Vpmg](#) *thee)
FORTRAN stub object destructor.
- VEXTERNNC int [Vpmg_fillco](#) ([Vpmg](#) *thee, [Vsurf_Meth](#) surfMeth, double splineWin, [Vchrg_Meth](#) chargeMeth, int useDielXMap, [Vgrid](#) *dielXMap, int useDielYMap, [Vgrid](#) *dielYMap, int useDielZMap, [Vgrid](#) *dielZMap, int useKappaMap, [Vgrid](#) *kappaMap, int usePotMap, [Vgrid](#) *potMap, int useChargeMap, [Vgrid](#) *chargeMap)
Fill the coefficient arrays prior to solving the equation.
- VEXTERNNC int [Vpmg_solve](#) ([Vpmg](#) *thee)
Solve the PBE using PMG.
- VEXTERNNC int [Vpmg_solveLaplace](#) ([Vpmg](#) *thee)
Solve Poisson's equation with a homogeneous Laplacian operator using the solvent dielectric constant. This solution is performed by a sine wave decomposition.
- VEXTERNNC double [Vpmg_energy](#) ([Vpmg](#) *thee, int extFlag)

- Get the total electrostatic energy.*

 - VEXTERNC double `Vpmg_qfEnergy` (`Vpmg *thee`, int extFlag)
- Get the "fixed charge" contribution to the electrostatic energy.*

 - VEXTERNC double `Vpmg_qfAtomEnergy` (`Vpmg *thee`, `Vatom *atom`)
- Get the per-atom "fixed charge" contribution to the electrostatic energy.*

 - VEXTERNC double `Vpmg_qmEnergy` (`Vpmg *thee`, int extFlag)
- Get the "mobile charge" contribution to the electrostatic energy.*

 - VEXTERNC double `Vpmg_dielEnergy` (`Vpmg *thee`, int extFlag)
- Get the "polarization" contribution to the electrostatic energy.*

 - VEXTERNC double `Vpmg_dielGradNorm` (`Vpmg *thee`)
- Get the integral of the gradient of the dielectric function.*

 - VEXTERNC int `Vpmg_force` (`Vpmg *thee`, double *force, int atomID, `Vsurf_Meth srfrm`, `Vchrg_Meth chgm`)
- Calculate the total force on the specified atom in units of $k_B T/AA$.*

 - VEXTERNC int `Vpmg_qfForce` (`Vpmg *thee`, double *force, int atomID, `Vchrg_Meth chgm`)
- Calculate the "charge-field" force on the specified atom in units of $k_B T/AA$.*

 - VEXTERNC int `Vpmg_dbForce` (`Vpmg *thee`, double *dbForce, int atomID, `Vsurf_Meth srfrm`)
- Calculate the dielectric boundary forces on the specified atom in units of $k_B T/AA$.*

 - VEXTERNC int `Vpmg_ibForce` (`Vpmg *thee`, double *force, int atomID, `Vsurf_Meth srfrm`)
- Calculate the osmotic pressure on the specified atom in units of $k_B T/AA$.*

 - VEXTERNC void `Vpmg_setPart` (`Vpmg *thee`, double lowerCorner[3], double upperCorner[3], int bflags[6])
- Set partition information which restricts the calculation of observables to a (rectangular) subset of the problem domain.*

 - VEXTERNC void `Vpmg_unsetPart` (`Vpmg *thee`)
- Remove partition restrictions.*

 - VEXTERNC int `Vpmg_fillArray` (`Vpmg *thee`, double *vec, `Vdata_Type type`, double parm, `Vhal_PBEType pbe-type`, `PBEparm *pbeparm`)
- Fill the specified array with accessibility values.*

 - VPUBLIC void `Vpmg_fieldSpline4` (`Vpmg *thee`, int atomID, double field[3])
- Computes the field at an atomic center using a stencil based on the first derivative of a 5th order B-spline.*

 - VEXTERNC double `Vpmg_qfPermanentMultipoleEnergy` (`Vpmg *thee`, int atomID)
- Computes the permanent multipole electrostatic hydration energy (the polarization component of the hydration energy currently computed in TINKER).*

 - VEXTERNC void `Vpmg_qfPermanentMultipoleForce` (`Vpmg *thee`, int atomID, double force[3], double torque[3])
- Computes the q-Phi Force for permanent multipoles based on 5th order B-splines.*

 - VEXTERNC void `Vpmg_ibPermanentMultipoleForce` (`Vpmg *thee`, int atomID, double force[3])
- Compute the ionic boundary force for permanent multipoles.*

 - VEXTERNC void `Vpmg_dbPermanentMultipoleForce` (`Vpmg *thee`, int atomID, double force[3])
- Compute the dielectric boundary force for permanent multipoles.*

 - VEXTERNC void `Vpmg_qfDirectPolForce` (`Vpmg *thee`, `Vgrid *perm`, `Vgrid *induced`, int atomID, double force[3], double torque[3])
- q-Phi direct polarization force between permanent multipoles and induced dipoles, which are induced by the sum of the permanent intramolecular field and the permanent reaction field.*

 - VEXTERNC void `Vpmg_qfNLDirectPolForce` (`Vpmg *thee`, `Vgrid *perm`, `Vgrid *nlInduced`, int atomID, double force[3], double torque[3])
- q-Phi direct polarization force between permanent multipoles and non-local induced dipoles based on 5th Order B-Splines. Keep in mind that the "non-local" induced dipoles are just a mathematical quantity that result from differentiation of the AMOEBA polarization energy.*

 - VEXTERNC void `Vpmg_ibDirectPolForce` (`Vpmg *thee`, `Vgrid *perm`, `Vgrid *induced`, int atomID, double force[3])
- Ionic boundary direct polarization force between permanent multipoles and induced dipoles, which are induced by the sum of the permanent intramolecular field and the permanent reaction field.*

- VEXTERNC void `Vpmg_ibNLDirectPolForce` (`Vpmg *thee`, `Vgrid *perm`, `Vgrid *nlInduced`, `int atomID`, `double force[3]`)
Ionic boundary direct polarization force between permanent multipoles and non-local induced dipoles based on 5th order. Keep in mind that the "non-local" induced dipoles are just a mathematical quantity that result from differentiation of the AMOEBA polarization energy.
- VEXTERNC void `Vpmg_dbDirectPolForce` (`Vpmg *thee`, `Vgrid *perm`, `Vgrid *induced`, `int atomID`, `double force[3]`)
Dielectric boundary direct polarization force between permanent multipoles and induced dipoles, which are induced by the sum of the permanent intramolecular field and the permanent reaction field.
- VEXTERNC void `Vpmg_dbNLDirectPolForce` (`Vpmg *thee`, `Vgrid *perm`, `Vgrid *nlInduced`, `int atomID`, `double force[3]`)
Dielectric boundary direct polarization force between permanent multipoles and non-local induced dipoles. Keep in mind that the "non-local" induced dipoles are just a mathematical quantity that result from differentiation of the AMOEBA polarization energy.
- VEXTERNC void `Vpmg_qfMutualPolForce` (`Vpmg *thee`, `Vgrid *induced`, `Vgrid *nlInduced`, `int atomID`, `double force[3]`)
Mutual polarization force for induced dipoles based on 5th order B-Splines. This force arises due to self-consistent convergence of the solute induced dipoles and reaction field.
- VEXTERNC void `Vpmg_ibMutualPolForce` (`Vpmg *thee`, `Vgrid *induced`, `Vgrid *nlInduced`, `int atomID`, `double force[3]`)
Ionic boundary mutual polarization force for induced dipoles based on 5th order B-Splines. This force arises due to self-consistent convergence of the solute induced dipoles and reaction field.
- VEXTERNC void `Vpmg_dbMutualPolForce` (`Vpmg *thee`, `Vgrid *induced`, `Vgrid *nlInduced`, `int atomID`, `double force[3]`)
Dielectric boundary mutual polarization force for induced dipoles based on 5th order B-Splines. This force arises due to self-consistent convergence of the solute induced dipoles and reaction field.
- VEXTERNC void `Vpmg_printColComp` (`Vpmg *thee`, `char path[72]`, `char title[72]`, `char mxtype[3]`, `int flag`)
Print out a column-compressed sparse matrix in Harwell-Boeing format.
- VPRIVATE void `bcolcomp` (`int *iparm`, `double *rparm`, `int *iwork`, `double *rwork`, `double *values`, `int *rowind`, `int *colptr`, `int *flag`)
Build a column-compressed matrix in Harwell-Boeing format.
- VPRIVATE void `bcolcomp2` (`int *iparm`, `double *rparm`, `int *nx`, `int *ny`, `int *nz`, `int *iz`, `int *ipc`, `double *rpc`, `double *ac`, `double *cc`, `double *values`, `int *rowind`, `int *colptr`, `int *flag`)
Build a column-compressed matrix in Harwell-Boeing format.
- VPRIVATE void `bcolcomp3` (`int *nx`, `int *ny`, `int *nz`, `int *ipc`, `double *rpc`, `double *ac`, `double *cc`, `double *values`, `int *rowind`, `int *colptr`, `int *flag`)
Build a column-compressed matrix in Harwell-Boeing format.
- VPRIVATE void `bcolcomp4` (`int *nx`, `int *ny`, `int *nz`, `int *ipc`, `double *rpc`, `double *oC`, `double *cc`, `double *oE`, `double *oN`, `double *uC`, `double *values`, `int *rowind`, `int *colptr`, `int *flag`)
Build a column-compressed matrix in Harwell-Boeing format.
- VPRIVATE void `pcolcomp` (`int *nrow`, `int *ncol`, `int *nnzero`, `double *values`, `int *rowind`, `int *colptr`, `char *path`, `char *title`, `char *mxtype`)
Print a column-compressed matrix in Harwell-Boeing format.
- VEXTERNC void `Vpackmg` (`int *iparm`, `double *rparm`, `size_t *nrwk`, `int *niwk`, `int *nx`, `int *ny`, `int *nz`, `int *nlev`, `int *nu1`, `int *nu2`, `int *mgkey`, `int *itmax`, `int *istop`, `int *ipcon`, `int *nonlin`, `int *mgsmoo`, `int *mgprol`, `int *mgcoar`, `int *mgsolv`, `int *mgdisc`, `int *iinfo`, `double *errtol`, `int *ipkey`, `double *omegal`, `double *omegan`, `int *irite`, `int *iperf`)
Print out a column-compressed sparse matrix in Harwell-Boeing format.

7.29.1 Detailed Description

A wrapper for Mike Holst's PMG multigrid code.

Note

Many of the routines and macros are borrowed from the [main.c](#) driver (written by Mike Holst) provided with the PMG code.

7.29.2 Typedef Documentation

7.29.2.1 Vpmg

```
typedef struct sVpmg Vpmg
```

Declaration of the Vpmg class as the Vpmg structure.

Definition at line 195 of file [vpmg.h](#).

7.29.3 Function Documentation

7.29.3.1 bcolcomp()

```
VPRIVATE void bcolcomp (
    int * iparm,
    double * rparm,
    int * iwork,
    double * rwork,
    double * values,
    int * rowind,
    int * colptr,
    int * flag )
```

Build a column-compressed matrix in Harwell-Boeing format.

Author

Tucker Beck [C Translation] Nathan Baker [Original] (mostly ripped off from Harwell-Boeing format documentation)Michael Schnieders)

Parameters

<i>iparm</i>	
<i>rparm</i>	
<i>iwork</i>	
<i>rwork</i>	
<i>values</i>	
<i>rowind</i>	
<i>colptr</i>	
<i>flag</i>	Operation selection parameter 0 = Use Poisson operator only 1 = Use linearization of full operation around current solution.

Definition at line 10741 of file [vpmg.c](#).

7.29.3.2 bcolcomp2()

```
VPRIVATE void bcolcomp2 (
    int * iparm,
```



```

double * rparm,
int * nx,
int * ny,
int * nz,
int * iz,
int * ipc,
double * rpc,
double * ac,
double * cc,
double * values,
int * rowind,
int * colptr,
int * flag )

```

Build a column-compressed matrix in Harwell-Boeing format.

Author

Tucker Beck [C Translation] Nathan Baker [Original] (mostly ripped off from Harwell-Boeing format documentation) Michael Schnieders)

Parameters

<i>iparm</i>	
<i>rparm</i>	
<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>iz</i>	
<i>ipc</i>	
<i>rpc</i>	
<i>ac</i>	
<i>cc</i>	
<i>values</i>	
<i>rowind</i>	
<i>colptr</i>	
<i>flag</i>	Operation selection parameter 0 = Use Poisson operator only 1 = Use linearization of full operation around current solution.

Definition at line [10795](#) of file [vpmg.c](#).

7.29.3.3 bcolcomp3()

```

VPRIVATE void bcolcomp3 (
    int * nx,
    int * ny,
    int * nz,
    int * ipc,
    double * rpc,
    double * ac,
    double * cc,
    double * values,
    int * rowind,
    int * colptr,

```

```
int * flag )
```

Build a column-compressed matrix in Harwell-Boeing format.

Author

Tucker Beck [C Translation] Nathan Baker [Original] (mostly ripped off from Harwell-Boeing format documentation)Michael Schnieders)

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>ipc</i>	
<i>rpc</i>	
<i>ac</i>	
<i>cc</i>	
<i>values</i>	
<i>rowind</i>	
<i>colptr</i>	
<i>flag</i>	

Definition at line [10831](#) of file [vpmg.c](#).

7.29.3.4 bcolcomp4()

```
VPRIVATE void bcolcomp4 (
    int * nx,
    int * ny,
    int * nz,
    int * ipc,
    double * rpc,
    double * oC,
    double * cc,
    double * oE,
    double * oN,
    double * uC,
    double * values,
    int * rowind,
    int * colptr,
    int * flag )
```

Build a column-compressed matrix in Harwell-Boeing format.

Author

Tucker Beck [C Translation] Nathan Baker [Original] (mostly ripped off from Harwell-Boeing format documentation)Michael Schnieders)

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	

Parameters

<i>ipc</i>	
<i>rpc</i>	
<i>oC</i>	
<i>cc</i>	
<i>oE</i>	
<i>oN</i>	
<i>uC</i>	
<i>values</i>	
<i>rowind</i>	
<i>colptr</i>	
<i>flag</i>	

Definition at line [10858](#) of file [vpmg.c](#).

7.29.3.5 pcolcomp()

```
VPRIVATE void pcolcomp (
    int * nrow,
    int * ncol,
    int * nnzero,
    double * values,
    int * rowind,
    int * colptr,
    char * path,
    char * title,
    char * mxtype )
```

Print a column-compressed matrix in Harwell-Boeing format.

Author

Tucker Beck [C Translation] Nathan Baker [Original] (mostly ripped off from Harwell-Boeing format documentation)Michael Schnieders)

Parameters

<i>nrow</i>	
<i>ncol</i>	
<i>nnzero</i>	
<i>values</i>	
<i>rowind</i>	
<i>colptr</i>	
<i>path</i>	
<i>title</i>	
<i>mxtype</i>	

Definition at line [11023](#) of file [vpmg.c](#).

7.29.3.6 Vpackmg()

```
VEXTERNC void Vpackmg (
```

```

    int * iparm,
    double * rparm,
    size_t * nrwk,
    int * niwk,
    int * nx,
    int * ny,
    int * nz,
    int * nlev,
    int * nul,
    int * nu2,
    int * mgkey,
    int * itmax,
    int * istop,
    int * ipcon,
    int * nonlin,
    int * mgsmoo,
    int * mgprol,
    int * mgcoar,
    int * mgsolv,
    int * mgdisc,
    int * iinfo,
    double * errtol,
    int * ipkey,
    double * omegal,
    double * omegan,
    int * irite,
    int * iperf )

```

Print out a column-compressed sparse matrix in Harwell-Boeing format.

Author

Nathan Baker

Bug Can this path variable be replaced with a Vio socket?

Definition at line 555 of file [mgsubd.c](#).

7.29.3.7 Vpmg_ctor()

```

VEXTERNC Vpmg * Vpmg_ctor (
    Vpmgp * parms,
    Vpbe * pbe,
    int focusFlag,
    Vpmg * pmgOLD,
    MGparm * mgparm,
    PBEparm_calcEnergy energyFlag )

```

Constructor for the Vpmg class (allocates new memory)

Author

Nathan Baker

Returns

Pointer to newly allocated Vpmg object

Parameters

<i>parms</i>	PMG parameter object
<i>pbe</i>	PBE-specific variables
<i>focusFlag</i>	1 for focusing, 0 otherwise
<i>pmgOLD</i>	Old Vpmg object to use for boundary conditions
<i>mgparm</i>	MGparm parameter object for boundary conditions
<i>energyFlag</i>	What types of energies to calculate

Definition at line 141 of file [vpmg.c](#).

7.29.3.8 Vpmg_ctor2()

```

VEXTERNC int Vpmg_ctor2 (
    Vpmg * thee,
    Vpmgp * parms,
    Vpbe * pbe,
    int focusFlag,
    Vpmg * pmgOLD,
    MGparm * mgparm,
    PBEparm_calcEnergy energyFlag )

```

FORTRAN stub constructor for the Vpmg class (uses previously-allocated memory)

Author

Nathan Baker

Returns

1 if successful, 0 otherwise

Note

this is common to both replace/noreplace options

The fortran replacement functions are run along side the old fortran functions. This is due to the use of common variables in the fortran sub-routines. Once the fortran code has been successfully excised, these functions will no longer need to be called in tandem, and the fortran version may be dropped

Parameters

<i>thee</i>	Memory location for object
<i>parms</i>	PMG parameter object
<i>pbe</i>	PBE-specific variables
<i>focusFlag</i>	1 for focusing, 0 otherwise
<i>pmgOLD</i>	Old Vpmg object to use for boundary conditions (can be VNULL if focusFlag = 0)
<i>mgparm</i>	MGparm parameter object for boundary conditions (can be VNULL if focusFlag = 0)
<i>energyFlag</i>	What types of energies to calculate (ignored if focusFlag = 0)

Definition at line 153 of file [vpmg.c](#).

7.29.3.9 Vpmg_dbDirectPolForce()

```
VEXTERNC void Vpmg_dbDirectPolForce (
    Vpmg * thee,
    Vgrid * perm,
    Vgrid * induced,
    int atomID,
    double force[3] )
```

Dielectric boundary direct polarization force between permanent multipoles and induced dipoles, which are induced by the sum of the permanent intramolecular field and the permanent reaction field.

Author

Michael Schnieders

Parameters

<i>thee</i>	Vpmg object
<i>perm</i>	Permanent multipole potential
<i>induced</i>	Induced dipole potential
<i>atomID</i>	Atom index
<i>force</i>	(returned) force

7.29.3.10 Vpmg_dbForce()

```
VEXTERNC int Vpmg_dbForce (
    Vpmg * thee,
    double * dbForce,
    int atomID,
    Vsurf_Meth srfm )
```

Calculate the dielectric boundary forces on the specified atom in units of $k_B T/AA$.

Author

Nathan Baker

Note

- Using the force evaluation methods of Im et al (Roux group), Comput Phys Commun, 111, 59–75 (1998). However, this gives the whole (self-interactions included) force – reaction field forces will have to be calculated at higher level.
- No contributions are made from higher levels of focusing.

Returns

1 if successful, 0 otherwise

Parameters

<i>thee</i>	Vpmg object
<i>dbForce</i>	3*sizeof(double) space to hold the dielectric boundary force in units of $k_B T/AA$
<i>atomID</i>	Valist ID of desired atom
<i>srfm</i>	Surface discretization method

Definition at line 6010 of file [vpmg.c](#).

7.29.3.11 Vpmg_dbMutualPolForce()

```
VEXTERNC void Vpmg_dbMutualPolForce (
    Vpmg * thee,
    Vgrid * induced,
    Vgrid * nlInduced,
    int atomID,
    double force[3] )
```

Dielectric boundary mutual polarization force for induced dipoles based on 5th order B-Splines. This force arises due to self-consistent convergence of the solute induced dipoles and reaction field.

Author

Michael Schnieders

Parameters

<i>thee</i>	Vpmg object
<i>induced</i>	Induced dipole potential
<i>nlInduced</i>	Non-local induced dipole potential
<i>atomID</i>	Atom index
<i>force</i>	(returned) force

7.29.3.12 Vpmg_dbNLDirectPolForce()

```
VEXTERNC void Vpmg_dbNLDirectPolForce (
    Vpmg * thee,
    Vgrid * perm,
    Vgrid * nlInduced,
    int atomID,
    double force[3] )
```

Dielectric boundary direct polarization force between permanent multipoles and non-local induced dipoles. Keep in mind that the "non-local" induced dipoles are just a mathematical quantity that result from differentiation of the AMOEBA polarization energy.

Author

Michael Schnieders

Parameters

<i>thee</i>	Vpmg object
<i>perm</i>	Permanent multipole potential
<i>nlInduced</i>	Non-local induced dipole potential
<i>atomID</i>	Atom index
<i>force</i>	(returned) force

7.29.3.13 Vpmg_dbPermanentMultipoleForce()

```

VEXTERNC void Vpmg_dbPermanentMultipoleForce (
    Vpmg * thee,
    int atomID,
    double force[3] )

```

Compute the dielectric boundary force for permanent multipoles.

Author

Michael Schnieders

Parameters

<i>thee</i>	Vpmg object
<i>atomID</i>	Atom index
<i>force</i>	(returned) force

7.29.3.14 Vpmg_dielEnergy()

```

VEXTERNC double Vpmg_dielEnergy (
    Vpmg * thee,
    int extFlag )

```

Get the "polarization" contribution to the electrostatic energy.

Using the solution at the finest mesh level, get the electrostatic energy due to the interaction of the mobile charges with the potential:

$$\int G = \frac{1}{2} \int \epsilon (\nabla u)^2 dx$$

where epsilon is the dielectric parameter and u(x) is the dimensionless electrostatic potential. The energy is scaled to units of $k_B T$.

Author

Nathan Baker

Note

The value of this observable may be modified by setting restrictions on the subdomain over which it is calculated. Such limits can be set via `Vpmg_setPart` and are generally useful for parallel runs.

Returns

The polarization electrostatic energy in units of $k_B T$.

Parameters

<i>thee</i>	Vpmg object
<i>extFlag</i>	If this was a focused calculation, include (1 – for serial calculations) or ignore (0 – for parallel calculations) energy contributions from outside the focusing domain

Definition at line 1279 of file `vpmg.c`.

7.29.3.15 Vpmg_dielGradNorm()

```
VEXTERNC double Vpmg_dielGradNorm (
    Vpmg * thee )
```

Get the integral of the gradient of the dielectric function.

Using the dielectric map at the finest mesh level, calculate the integral of the norm of the dielectric function gradient routines of Im et al (see Vpmg_dbForce for reference):

$$\int \nabla \epsilon \, dx$$
 where epsilon is the dielectric parameter.
 The integral is returned in units of A^2 .

Author

Nathan Baker restrictions on the subdomain over which it is calculated. Such limits can be set via Vpmg_setPart and are generally useful for parallel runs.

Returns

The integral in units of A^2 .

Parameters

<i>thee</i>	Vpmg object
-------------	-------------

Definition at line 1342 of file vpmg.c.

7.29.3.16 Vpmg_dtor()

```
VEXTERNC void Vpmg_dtor (
    Vpmg ** thee )
```

Object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to memory location of object to be destroyed
-------------	--

Definition at line 561 of file vpmg.c.

7.29.3.17 Vpmg_dtor2()

```
VEXTERNC void Vpmg_dtor2 (
    Vpmg * thee )
```

FORTTRAN stub object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to object to be destroyed
-------------	-----------------------------------

Definition at line 571 of file [vpmg.c](#).

7.29.3.18 Vpmg_energy()

```
VEXTERNC double Vpmg_energy (
    Vpmg * thee,
    int extFlag )
```

Get the total electrostatic energy.

Author

Nathan Baker

Note

The value of this observable may be modified by setting restrictions on the subdomain over which it is calculated. Such limits can be set via `Vpmg_setPart` and are generally useful for parallel runs.

Returns

The electrostatic energy in units of $k_B T$.

Parameters

<i>thee</i>	Vpmg object
<i>extFlag</i>	If this was a focused calculation, include (1 – for serial calculations) or ignore (0 – for parallel calculations) energy contributions from outside the focusing domain

Definition at line 1248 of file [vpmg.c](#).

7.29.3.19 Vpmg_fieldSpline4()

```
VPUBLIC void Vpmg_fieldSpline4 (
    Vpmg * thee,
    int atomID,
    double field[3] )
```

Computes the field at an atomic center using a stencil based on the first derivative of a 5th order B-spline.

Author

Michael Schnieders

Parameters

<i>thee</i>	Vpmg object
<i>atomID</i>	Atom index
<i>field</i>	The (returned) electric field

7.29.3.20 Vpmg_fillArray()

```

VEXTERNC int Vpmg_fillArray (
    Vpmg * thee,
    double * vec,
    Vdata_Type type,
    double parm,
    Vhal_PBEType pbetype,
    PBEparm * pbeparm )

```

Fill the specified array with accessibility values.

Author

Nathan Baker

Returns

1 if successful, 0 otherwise

Parameters

<i>thee</i>	Vpmg object
<i>vec</i>	A nx*ny*nz*sizeof(double) array to contain the values to be written
<i>type</i>	What to write
<i>parm</i>	Parameter for data type definition (if needed)
<i>pbetype</i>	Parameter for PBE type (if needed)
<i>pbeparm</i>	Pass in the PBE parameters (if needed)

Definition at line 892 of file [vpmg.c](#).

7.29.3.21 Vpmg_fillco()

```

VEXTERNC int Vpmg_fillco (
    Vpmg * thee,
    Vsurf_Meth surfMeth,
    double splineWin,
    Vchrg_Meth chargeMeth,
    int useDielXMap,
    Vgrid * dielXMap,
    int useDielYMap,
    Vgrid * dielYMap,
    int useDielZMap,
    Vgrid * dielZMap,
    int useKappaMap,
    Vgrid * kappaMap,
    int usePotMap,
    Vgrid * potMap,
    int useChargeMap,
    Vgrid * chargeMap )

```

Fill the coefficient arrays prior to solving the equation.

Author

Nathan Baker

Returns

1 if successful, 0 otherwise

Bug useDielMap could only be passed once, not three times, to this function - why not just once? that's what the call in [routines.c](#) ends up doing - just passing useDielMap three times. - P. Ellis 11/3/11

Parameters

<i>thee</i>	Vpmg object
<i>surfMeth</i>	Surface discretization method
<i>splineWin</i>	Spline window (in A) for surfMeth = VSM_SPLINE
<i>chargeMeth</i>	Charge discretization method
<i>useDielXMap</i>	Boolean to use dielectric map argument
<i>dielXMap</i>	External dielectric map
<i>useDielYMap</i>	Boolean to use dielectric map argument
<i>dielYMap</i>	External dielectric map
<i>useDielZMap</i>	Boolean to use dielectric map argument
<i>dielZMap</i>	External dielectric map
<i>useKappaMap</i>	Boolean to use kappa map argument
<i>kappaMap</i>	External kappa map
<i>usePotMap</i>	Boolean to use potential map argument
<i>potMap</i>	External potential map
<i>useChargeMap</i>	Boolean to use charge map argument
<i>chargeMap</i>	External charge map

Definition at line 5655 of file [vpmg.c](#).

7.29.3.22 Vpmg_force()

```

VEXTERNC int Vpmg_force (
    Vpmg * thee,
    double * force,
    int atomID,
    Vsurf_Meth srfm,
    Vchrg_Meth chgm )

```

Calculate the total force on the specified atom in units of k_B T/AA.

Author

Nathan Baker

Note

- Using the force evaluation methods of Im et al (Roux group), Comput Phys Commun, 111, 59–75 (1998). However, this gives the whole (self-interactions included) force – reaction field forces will have to be calculated at higher level.
- No contributions are made from higher levels of focusing.

Returns

1 if successful, 0 otherwise

Parameters

<i>thee</i>	Vpmg object
<i>force</i>	3*sizeof(double) space to hold the force in units of k _B T/Å
<i>atomID</i>	Valist ID of desired atom
<i>srfm</i>	Surface discretization method
<i>chgm</i>	Charge discretization method

Definition at line 5822 of file [vpmg.c](#).

7.29.3.23 Vpmg_ibDirectPolForce()

```
VEXTERNC void Vpmg_ibDirectPolForce (
    Vpmg * thee,
    Vgrid * perm,
    Vgrid * induced,
    int atomID,
    double force[3] )
```

Ionic boundary direct polarization force between permanent multipoles and induced dipoles, which are induced by the sum of the permanent intramolecular field and the permanent reaction field.

Author

Michael Schnieders

Parameters

<i>thee</i>	Vpmg object
<i>perm</i>	Permanent multipole potential
<i>induced</i>	Induced dipole potential
<i>atomID</i>	Atom index
<i>force</i>	(returned) force

7.29.3.24 Vpmg_ibForce()

```
VEXTERNC int Vpmg_ibForce (
    Vpmg * thee,
    double * force,
    int atomID,
    Vsurf_Meth srfm )
```

Calculate the osmotic pressure on the specified atom in units of k_B T/Å.

Author

Nathan Baker

Note

- Using the force evaluation methods of Im et al (Roux group), Comput Phys Commun, 111, 59–75 (1998). However, this gives the whole (self-interactions included) force – reaction field forces will have to be calculated at higher level.
- No contributions are made from higher levels of focusing.

Returns

1 if successful, 0 otherwise

Parameters

<i>thee</i>	Vpmpg object
<i>force</i>	3*sizeof(double) space to hold the boundary force in units of $k_B T/AA$
<i>atomID</i>	Valist ID of desired atom
<i>srfm</i>	Surface discretization method

Definition at line 5845 of file [vpmpg.c](#).

7.29.3.25 Vpmpg_ibMutualPolForce()

```
VEXTERNC void Vpmpg_ibMutualPolForce (
    Vpmpg * thee,
    Vgrid * induced,
    Vgrid * nlInduced,
    int atomID,
    double force[3] )
```

Ionic boundary mutual polarization force for induced dipoles based on 5th order B-Splines. This force arises due to self-consistent convergence of the solute induced dipoles and reaction field.

Author

Michael Schnieders

Parameters

<i>thee</i>	Vpmpg object
<i>induced</i>	Induced dipole potential
<i>nlInduced</i>	Non-local induced dipole potential
<i>atomID</i>	Atom index
<i>force</i>	(returned) force

7.29.3.26 Vpmpg_ibNLDirectPolForce()

```
VEXTERNC void Vpmpg_ibNLDirectPolForce (
    Vpmpg * thee,
    Vgrid * perm,
    Vgrid * nlInduced,
    int atomID,
    double force[3] )
```

Ionic boundary direct polarization force between permanent multipoles and non-local induced dipoles based on 5th order Keep in mind that the "non-local" induced dipoles are just a mathematical quantity that result from differentiation of the AMOEBA polarization energy.

Author

Michael Schnieders

Parameters

<i>thee</i>	Vpmg object
<i>perm</i>	Permanent multipole potential
<i>nInduced</i>	Induced dipole potential
<i>atomID</i>	Atom index
<i>force</i>	(returned) force

7.29.3.27 Vpmg_ibPermanentMultipoleForce()

```
VEXTERNC void Vpmg_ibPermanentMultipoleForce (
    Vpmg * thee,
    int atomID,
    double force[3] )
```

Compute the ionic boundary force for permanent multipoles.

Author

Michael Schnieders

Parameters

<i>thee</i>	Vpmg object
<i>atomID</i>	Atom index
<i>force</i>	(returned) force

7.29.3.28 Vpmg_memChk()

```
VEXTERNC unsigned long int Vpmg_memChk (
    Vpmg * thee )
```

Return the memory used by this structure (and its contents) in bytes.

Author

Nathan Baker

Returns

The memory used by this structure and its contents in bytes

Parameters

<i>thee</i>	Object for memory check
-------------	-------------------------

Definition at line 79 of file [vpmg.c](#).

7.29.3.29 Vpmg_printColComp()

```
VEXTERNC void Vpmg_printColComp (
    Vpmg * thee,
    char path[72],
```

```
char title[72],
char mxtype[3],
int flag )
```

Print out a column-compressed sparse matrix in Harwell-Boeing format.

Author

Nathan Baker

Bug Can this path variable be replaced with a Vio socket?

Parameters

<i>thee</i>	Vpmg object
<i>path</i>	The file to which the matrix is to be written
<i>title</i>	The title of the matrix
<i>mxtype</i>	The type of REAL-valued matrix, a 3-character string of the form "R_A" where the '_' can be one of: <ul style="list-style-type: none"> • S: symmetric matrix • U: unsymmetric matrix • H: Hermitian matrix • Z: skew-symmetric matrix • R: rectangular matrix
<i>flag</i>	The operator to compress: <ul style="list-style-type: none"> • 0: Poisson operator • 1: Linearization of the full Poisson-Boltzmann operator around the current solution

Definition at line 87 of file [vpmg.c](#).

7.29.3.30 Vpmg_qfAtomEnergy()

```
VEXTERNC double Vpmg_qfAtomEnergy (
    Vpmg * thee,
    Vatom * atom )
```

Get the per-atom "fixed charge" contribution to the electrostatic energy.

Using the solution at the finest mesh level, get the electrostatic energy due to the interaction of the fixed charges with the potential:

$$G = qu(r),$$

where q is the charge and r is the location of the atom of interest. The result is returned in units of $k_B T$. Clearly, no self-interaction terms are removed. A factor a 1/2 has to be included to convert this to a real energy.

Author

Nathan Baker

Note

The value of this observable may be modified by setting restrictions on the subdomain over which it is calculated. Such limits can be set via `Vpmg_setPart` and are generally useful for parallel runs.

Returns

The fixed charge electrostatic energy in units of $k_B T$.

Parameters

<i>thee</i>	The Vpmg object
<i>atom</i>	The atom for energy calculations

Definition at line 1791 of file [vpmg.c](#).

7.29.3.31 Vpmg_qfDirectPolForce()

```
VEXTERNC void Vpmg_qfDirectPolForce (
    Vpmg * thee,
    Vgrid * perm,
    Vgrid * induced,
    int atomID,
    double force[3],
    double torque[3] )
```

q-Phi direct polarization force between permanent multipoles and induced dipoles, which are induced by the sum of the permanent intramolecular field and the permanent reaction field.

Author

Michael Schnieders

Parameters

<i>thee</i>	Vpmg object
<i>perm</i>	Permanent multipole potential
<i>induced</i>	Induced dipole potential
<i>atomID</i>	Atom index
<i>force</i>	(returned) force
<i>torque</i>	(returned) torque

7.29.3.32 Vpmg_qfEnergy()

```
VEXTERNC double Vpmg_qfEnergy (
    Vpmg * thee,
    int extFlag )
```

Get the "fixed charge" contribution to the electrostatic energy.

Using the solution at the finest mesh level, get the electrostatic energy due to the interaction of the fixed charges with the potential: $\sum_i q_i u(r_i)$ and return the result in units of $k_B T$. Clearly, no self-interaction terms are removed. A factor a 1/2 has to be included to convert this to a real energy.

Author

Nathan Baker

Note

The value of this observable may be modified by setting restrictions on the subdomain over which it is calculated. Such limits can be set via `Vpmg_setPart` and are generally useful for parallel runs.

Returns

The fixed charge electrostatic energy in units of $k_B T$.

Parameters

<i>thee</i>	Vpmg object
<i>extFlag</i>	If this was a focused calculation, include (1 – for serial calculations) or ignore (0 – for parallel calculations) energy contributions from outside the focusing domain

Definition at line 1687 of file `vpmg.c`.

7.29.3.33 Vpmg_qfForce()

```

VEXTERNC int Vpmg_qfForce (
    Vpmg * thee,
    double * force,
    int atomID,
    Vchrg_Meth chgm )

```

Calculate the "charge-field" force on the specified atom in units of $k_B T/AA$.

Author

Nathan Baker

Note

- Using the force evaluation methods of Im et al (Roux group), Comput Phys Commun, 111, 59–75 (1998). However, this gives the whole (self-interactions included) force – reaction field forces will have to be calculated at higher level.
- No contributions are made from higher levels of focusing.

Returns

1 if successful, 0 otherwise

Parameters

<i>thee</i>	Vpmg object
<i>force</i>	3*sizeof(double) space to hold the force in units of $k_B T/A$
<i>atomID</i>	Valist ID of desired atom
<i>chgm</i>	Charge discretization method

Definition at line 6267 of file `vpmg.c`.

7.29.3.34 Vpmg_qfMutualPolForce()

```

VEXTERNC void Vpmg_qfMutualPolForce (

```

```

Vpmg * thee,
Vgrid * induced,
Vgrid * nlInduced,
int atomID,
double force[3] )

```

Mutual polarization force for induced dipoles based on 5th order B-Splines. This force arises due to self-consistent convergence of the solute induced dipoles and reaction field.

Author

Michael Schnieders

Parameters

<i>thee</i>	Vpmg object
<i>induced</i>	Induced dipole potential
<i>nlInduced</i>	Non-local induced dipole potential
<i>atomID</i>	Atom index
<i>force</i>	(returned) force

7.29.3.35 Vpmg_qfNLDirectPolForce()

```

VEXTERNC void Vpmg_qfNLDirectPolForce (
    Vpmg * thee,
    Vgrid * perm,
    Vgrid * nlInduced,
    int atomID,
    double force[3],
    double torque[3] )

```

q-Phi direct polarization force between permanent multipoles and non-local induced dipoles based on 5th Order B-Splines. Keep in mind that the "non-local" induced dipoles are just a mathematical quantity that result from differentiation of the AMOEBA polarization energy.

Author

Michael Schnieders

Parameters

<i>thee</i>	Vpmg object
<i>perm</i>	Permanent multipole potential
<i>nlInduced</i>	Non-local induced dipole potential
<i>atomID</i>	Atom index
<i>force</i>	(returned) force
<i>torque</i>	(returned) torque

7.29.3.36 Vpmg_qfPermanentMultipoleEnergy()

```

VEXTERNC double Vpmg_qfPermanentMultipoleEnergy (
    Vpmg * thee,
    int atomID )

```

Computes the permanent multipole electrostatic hydration energy (the polarization component of the hydration energy currently computed in TINKER).

Author

Michael Schnieders

Returns

The permanent multipole electrostatic hydration energy

Parameters

<i>thee</i>	Vpmg object
<i>atomID</i>	Atom index

7.29.3.37 Vpmg_qfPermanentMultipoleForce()

```

VEXTERNC void Vpmg_qfPermanentMultipoleForce (
    Vpmg * thee,
    int atomID,
    double force[3],
    double torque[3] )

```

Computes the q-Phi Force for permanent multipoles based on 5th order B-splines.

Author

Michael Schnieders

Parameters

<i>thee</i>	Vpmg object
<i>atomID</i>	Atom index
<i>force</i>	(returned) force
<i>torque</i>	(returned) torque

7.29.3.38 Vpmg_qmEnergy()

```

VEXTERNC double Vpmg_qmEnergy (
    Vpmg * thee,
    int extFlag )

```

Get the "mobile charge" contribution to the electrostatic energy.

Using the solution at the finest mesh level, get the electrostatic energy due to the interaction of the mobile charges with the potential:

$$\int \left[G = \frac{1}{4} I_s \sum_i c_i q_i^2 \int \kappa^2(x) e^{-q_i u(x)} dx \right]$$

for the NPBE and

$$\int \left[G = \frac{1}{2} \int \overline{\kappa^2(x)} u^2(x) dx \right]$$

for the LPBE. Here i denotes the counterion species, I_s is the bulk ionic strength, $\kappa^2(x)$ is the modified Debye-Huckel parameter, c_i is the concentration of species i , q_i is the charge of

species i , and $u(x)$ is the dimensionless electrostatic potential. The energy is scaled to units of $k_B T$.

Author

Nathan Baker

Note

The value of this observable may be modified by setting restrictions on the subdomain over which it is calculated. Such limits can be set via `Vpmg_setPart` and are generally useful for parallel runs.

Returns

The mobile charge electrostatic energy in units of $k_B T$.

Parameters

<i>thee</i>	Vpmg object
<i>extFlag</i>	If this was a focused calculation, include (1 – for serial calculations) or ignore (0 – for parallel calculations) energy contributions from outside the focusing domain

Definition at line 1386 of file `vpmg.c`.

7.29.3.39 Vpmg_setPart()

```

VEXTERNC void Vpmg_setPart (
    Vpmg * thee,
    double lowerCorner[3],
    double upperCorner[3],
    int bflags[6] )

```

Set partition information which restricts the calculation of observables to a (rectangular) subset of the problem domain.

Author

Nathan Baker

Parameters

<i>thee</i>	Vpmg object
<i>lowerCorner</i>	Partition lower corner
<i>upperCorner</i>	Partition upper corner
<i>bflags</i>	Booleans indicating whether a particular processor is on the boundary with another partition. 0 if the face is not bounded (next to) another partition, and 1 otherwise.

Definition at line 627 of file `vpmg.c`.

7.29.3.40 Vpmg_solve()

```

VEXTERNC int Vpmg_solve (
    Vpmg * thee )

```

Solve the PBE using PMG.

Author

Nathan Baker

Returns

1 if successful, 0 otherwise

Parameters

<i>thee</i>	Vpmg object
-------------	-------------

Definition at line 401 of file [vpmg.c](#).

7.29.3.41 Vpmg_solveLaplace()

```
VEXTERNC int Vpmg_solveLaplace (  
    Vpmg * thee )
```

Solve Poisson's equation with a homogeneous Laplacian operator using the solvent dielectric constant. This solution is performed by a sine wave decomposition.

Author

Nathan Baker

Returns

1 if successful, 0 otherwise

Note

This function is really only for testing purposes as the PMG multigrid solver can solve the homogeneous system much more quickly. Perhaps we should implement an FFT version at some point...

Parameters

<i>thee</i>	Vpmg object
-------------	-------------

Definition at line 7042 of file [vpmg.c](#).

7.29.3.42 Vpmg_unsetPart()

```
VEXTERNC void Vpmg_unsetPart (  
    Vpmg * thee )
```

Remove partition restrictions.

Author

Nathan Baker

Parameters

<i>thee</i>	Vpmg object
-------------	-------------

Definition at line 872 of file [vpmg.c](#).

7.30 Vpmgp class

Parameter structure for Mike Holst's PMGP code.

Files

- file [vpmgp.c](#)
Class Vpmgp methods.
- file [vpmgp.h](#)
Contains declarations for class Vpmgp.

Data Structures

- struct [sVpmgp](#)
Contains public data members for Vpmgp class/module.

Typedefs

- typedef struct [sVpmgp](#) Vpmgp
Declaration of the Vpmgp class as the sVpmgp structure.

Functions

- VEXTERNC [Vpmgp](#) * [Vpmgp_ctor](#) ([MGparm](#) *mgparm)
Construct PMG parameter object and initialize to default values.
- VEXTERNC int [Vpmgp_ctor2](#) ([Vpmgp](#) *thee, [MGparm](#) *mgparm)
FORTTRAN stub to construct PMG parameter object and initialize to default values.
- VEXTERNC void [Vpmgp_dtor](#) ([Vpmgp](#) **thee)
Object destructor.
- VEXTERNC void [Vpmgp_dtor2](#) ([Vpmgp](#) *thee)
FORTTRAN stub for object destructor.
- VEXTERNC void [Vpmgp_size](#) ([Vpmgp](#) *thee)
Determine array sizes and parameters for multigrid solver.
- VEXTERNC void [Vpmgp_makeCoarse](#) (int numLevel, int nxOld, int nyOld, int nzOld, int *nxNew, int *nyNew, int *nzNew)
Coarsen the grid by the desired number of levels and determine the resulting numbers of grid points.

7.30.1 Detailed Description

Parameter structure for Mike Holst's PMGP code.

Note

Variables and many default values taken directly from PMG

7.30.2 Typedef Documentation

7.30.2.1 Vpmgp

```
typedef struct sVpmgp Vpmgp
```

Declaration of the Vpmgp class as the [sVpmgp](#) structure.

Definition at line 204 of file [vpmgp.h](#).

7.30.3 Function Documentation

7.30.3.1 Vpmgp_ctor()

```

VEXTERNC Vpmgp * Vpmgp_ctor (
    MGparm * mgparm )

```

Construct PMG parameter object and initialize to default values.

Author

Nathan Baker

Parameters

<i>mgparm</i>	MGParm object containing parameters to be used in setup
---------------	---

Returns

Newly allocated and initialized Vpmgp object

Definition at line 76 of file [vpmgp.c](#).

7.30.3.2 Vpmgp_ctor2()

```

VEXTERNC int Vpmgp_ctor2 (
    Vpmgp * thee,
    MGparm * mgparm )

```

FORTTRAN stub to construct PMG parameter object and initialize to default values.

Author

Nathan Baker

Parameters

<i>thee</i>	Newly allocated PMG object
<i>mgparm</i>	MGParm object containing parameters to be used in setup

Returns

1 if successful, 0 otherwise

Definition at line 93 of file [vpmgp.c](#).

7.30.3.3 Vpmgp_dtor()

```

VEXTERNC void Vpmgp_dtor (
    Vpmgp ** thee )

```

Object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to memory location for Vpmgp object
-------------	---

Definition at line 178 of file [vpmgp.c](#).

7.30.3.4 Vpmgp_dtor2()

```
VEXTERNC void Vpmgp_dtor2 (
    Vpmgp * thee )
```

FORTTRAN stub for object destructor.

Author

Nathan Baker

Parameters

<i>thee</i>	Pointer to Vpmgp object
-------------	-------------------------

Definition at line 193 of file [vpmgp.c](#).

7.30.3.5 Vpmgp_makeCoarse()

```
VEXTERNC void Vpmgp_makeCoarse (
    int numLevel,
    int nxOld,
    int nyOld,
    int nzOld,
    int * nxNew,
    int * nyNew,
    int * nzNew )
```

Coarsen the grid by the desired number of levels and determine the resulting numbers of grid points.

Author

Mike Holst and Nathan Baker

Parameters

<i>numLevel</i>	Number of levels to coarsen
<i>nxOld</i>	Number of old grid points in this direction
<i>nyOld</i>	Number of old grid points in this direction
<i>nzOld</i>	Number of old grid points in this direction
<i>nxNew</i>	Number of new grid points in this direction
<i>nyNew</i>	Number of new grid points in this direction
<i>nzNew</i>	Number of new grid points in this direction

Definition at line 312 of file [vpmgp.c](#).

7.30.3.6 Vpmgp_size()

```
VEXTERNC void Vpmgp_size (
```

`Vpmgp * thee)`

Determine array sizes and parameters for multigrid solver.

Author

Mike Holst and Nathan Baker

Parameters

<code>thee</code>	Object to be sized
-------------------	--------------------

Definition at line 196 of file `vpmgp.c`.

7.31 C translation of Holst group PMG code

C translation of Holst group PMG code.

Macros

- `#define HARMO2(a, b) (2.0 * (a) * (b) / ((a) + (b)))`
Multigrid subroutines.
- `#define MAXIONS 50`
Specifies the PDE definition for PMG to solve.

Functions

- `VPUBLIC void VbuildA (int *nx, int *ny, int *nz, int *ipkey, int *mgdisc, int *numdia, int *ipc, double *rpc, double *ac, double *cc, double *fc, double *xf, double *yf, double *zf, double *gxcf, double *gycf, double *gzcf, double *a1cf, double *a2cf, double *a3cf, double *ccf, double *fcf)`
Build the Laplacian.
- `VPUBLIC void Vbuildband (int *key, int *nx, int *ny, int *nz, int *ipc, double *rpc, double *ac, int *ipcB, double *rpcB, double *acB)`
Banded matrix builder.
- `VEXTERN void Vbuildband1_7 (int *nx, int *ny, int *nz, int *ipc, double *rpc, double *oC, double *oE, double *oN, double *uC, int *ipcB, double *rpcB, double *acB, int *n, int *m, int *lda)`
Build the operator in banded form given the 7-diagonal form.
- `VEXTERN void Vbuildband1_27 (int *nx, int *ny, int *nz, int *ipc, double *rpc, double *oC, double *oE, double *oN, double *uC, double *oNE, double *oNW, double *uE, double *uW, double *uN, double *uS, double *uNE, double *uNW, double *uSE, double *uSW, int *ipcB, double *rpcB, double *acB, int *n, int *m, int *lda)`
Build the operator in banded form given the 27-diagonal form.
- `VPUBLIC void VbuildG (int *nxf, int *nyf, int *nzf, int *nxc, int *nyc, int *nzc, int *numdia, double *pcFF, double *acFF, double *ac)`
Build Galerkin matrix structures.
- `VEXTERN void VbuildG_1 (int *nxf, int *nyf, int *nzf, int *nx, int *ny, int *nz, double *oPC, double *oPN, double *oPS, double *oPE, double *oPW, double *oPNE, double *oPNW, double *oPSE, double *oPSW, double *uPC, double *uPN, double *uPS, double *uPE, double *uPW, double *uPNE, double *uPNW, double *uPSE, double *uPSW, double *dPC, double *dPN, double *dPS, double *dPE, double *dPW, double *dPNE, double *dPNW, double *dPSE, double *dPSW, double *oC, double *XoC, double *XoE, double *XoN, double *XuC, double *XoNE, double *XoNW, double *XuE, double *XuW, double *XuN, double *XuS, double *XuNE, double *XuNW, double *XuSE, double *XuSW)`
Computes a 27-point galerkin coarse grid matrix from a 1-point (i.e., diagonal) fine grid matrix.

- VEXTERNC void **VbuildG_7** (int *nxf, int *nyf, int *nzf, int *nx, int *ny, int *nz, double *oPC, double *oPN, double *oPS, double *oPE, double *oPW, double *oPNE, double *oPNW, double *oPSE, double *oPSW, double *uPC, double *uPN, double *uPS, double *uPE, double *uPW, double *uPNE, double *uPNW, double *uPSE, double *uPSW, double *dPC, double *dPN, double *dPS, double *dPE, double *dPW, double *dPNE, double *dPNW, double *dPSE, double *dPSW, double *oC, double *oE, double *oN, double *uC, double *XoC, double *XoE, double *XoN, double *XuC, double *XoNE, double *XoNW, double *XuE, double *XuW, double *XuN, double *XuS, double *XuNE, double *XuNW, double *XuSE, double *XuSW)

Computes a 27-point galerkin coarse grid matrix from a 7-point fine grid matrix.

- VEXTERNC void **VbuildG_27** (int *nxf, int *nyf, int *nzf, int *nx, int *ny, int *nz, double *oPC, double *oPN, double *oPS, double *oPE, double *oPW, double *oPNE, double *oPNW, double *oPSE, double *oPSW, double *uPC, double *uPN, double *uPS, double *uPE, double *uPW, double *uPNE, double *uPNW, double *uPSE, double *uPSW, double *dPC, double *dPN, double *dPS, double *dPE, double *dPW, double *dPNE, double *dPNW, double *dPSE, double *dPSW, double *oC, double *oE, double *oN, double *uC, double *oNE, double *oNW, double *uE, double *uW, double *uN, double *uS, double *uNE, double *uNW, double *uSE, double *uSW, double *XoC, double *XoE, double *XoN, double *XuC, double *XoNE, double *XoNW, double *XuE, double *XuW, double *XuN, double *XuS, double *XuNE, double *XuNW, double *XuSE, double *XuSW)

Compute a 27-point galerkin coarse grid matrix from a 27-point fine grid matrix.

- VPUBLIC void **VbuildP** (int *nxf, int *nyf, int *nzf, int *nxc, int *nyc, int *nzc, int *mgprol, int *ipc, double *rpc, double *pc, double *ac, double *xf, double *yf, double *zf)

Builds prolongation matrix.

- VPUBLIC void **Vcghs** (int *nx, int *ny, int *nz, int *ipc, double *rpc, double *ac, double *cc, double *fc, double *x, double *p, double *ap, double *r, int *itmax, int *iters, double *errtol, double *omega, int *iresid, int *iadjoint)

A collection of useful low-level routines (timing, etc).

- VPUBLIC void **Vgsrb** (int *nx, int *ny, int *nz, int *ipc, double *rpc, double *ac, double *cc, double *fc, double *x, double *w1, double *w2, double *r, int *itmax, int *iters, double *errtol, double *omega, int *iresid, int *iadjoint)

Guass-Seidel solver.

- VPUBLIC void **Vmatvec** (int *nx, int *ny, int *nz, int *ipc, double *rpc, double *ac, double *cc, double *x, double *y)

Matrix-vector multiplication routines.

- VEXTERNC void **Vnmatvec** (int *nx, int *ny, int *nz, int *ipc, double *rpc, double *ac, double *cc, double *x, double *y, double *w1)

Break the matrix data-structure into diagonals and then call the matrix-vector routine.

- VEXTERNC void **Vmresid** (int *nx, int *ny, int *nz, int *ipc, double *rpc, double *ac, double *cc, double *fc, double *x, double *r)

Break the matrix data-structure into diagonals and then call the residual routine.

- VEXTERNC void **Vnmresid** (int *nx, int *ny, int *nz, int *ipc, double *rpc, double *ac, double *cc, double *fc, double *x, double *r, double *w1)

Break the matrix data-structure into diagonals and then call the residual routine.

- VEXTERNC void **Vrestrc** (int *nxf, int *nyf, int *nzf, int *nxc, int *nyc, int *nzc, double *xin, double *xout, double *pc)

Apply the restriction operator.

- VEXTERNC void **VinterpPMG** (int *nxc, int *nyc, int *nzc, int *nxf, int *nyf, int *nzf, double *xin, double *xout, double *pc)

Apply the prolongation operator.

- VEXTERNC void **Vextrac** (int *nxf, int *nyf, int *nzf, int *nxc, int *nyc, int *nzc, double *xin, double *xout)

Simple injection of a fine grid function into coarse grid.

- VEXTERNC void **Vmvcs** (int *nx, int *ny, int *nz, double *x, int *iz, double *w0, double *w1, double *w2, double *w3, int *istop, int *itmax, int *iters, int *ierror, int *nlev, int *ilev, int *nlev_real, int *mgsolv, int *iok, int *iinfo, double *epsilon, double *errtol, double *omega, int *nu1, int *nu2, int *mgsmoo, int *ipc, double *rpc, double *pc, double *ac, double *cc, double *fc, double *tru)

MG helper functions.

- VPUBLIC void **Vmgdriv** (int *iparm, double *rparm, int *iwork, double *rwork, double *u, double *xf, double *yf, double *zf, double *gxcf, double *gycf, double *gzcf, double *a1cf, double *a2cf, double *a3cf, double *ccf, double *fcf, double *tcf)

Multilevel solver driver.

- VEXTERNC void **Vmgdriv2** (int *iparm, double *rparm, int *nx, int *ny, int *nz, double *u, int *iz, int *ipc, double *rpc, double *pc, double *ac, double *cc, double *fc, double *xf, double *yf, double *zf, double *gxcf, double *gycf, double *gzcf, double *a1cf, double *a2cf, double *a3cf, double *ccf, double *fcf, double *tcf)

Solves the pde using the multi-grid method.

- VEXTERNC void **Vmgisz** (int *mgcoar, int *mgdisc, int *mgsolv, int *nx, int *ny, int *nz, int *nlev, int *nxc, int *nyc, int *nzc, int *nf, int *nc, int *narr, int *narrc, int *n_rpc, int *n_iz, int *n_ipc, int *iretot, int *iintot)

This routine computes the required sizes of the real and integer work arrays for the multigrid code. these two sizes are a (complicated) function of input parameters.

- VPUBLIC void **Vfmvfas** (int *nx, int *ny, int *nz, double *x, int *iz, double *w0, double *w1, double *w2, double *w3, double *w4, int *istop, int *itmax, int *iters, int *ierror, int *nlev, int *ilev, int *nlev_real, int *mgsolv, int *iok, int *iinfo, double *epsiln, double *errtol, double *omega, int *nu1, int *nu2, int *mgsmoo, int *ipc, double *rpc, double *pc, double *ac, double *cc, double *fc, double *tru)

Multigrid nonlinear solve iteration routine.

- VEXTERNC void **Vmvfas** (int *nx, int *ny, int *nz, double *x, int *iz, double *w0, double *w1, double *w2, double *w3, double *w4, int *istop, int *itmax, int *iters, int *ierror, int *nlev, int *ilev, int *nlev_real, int *mgsolv, int *iok, int *iinfo, double *epsiln, double *errtol, double *omega, int *nu1, int *nu2, int *mgsmoo, int *ipc, double *rpc, double *pc, double *ac, double *cc, double *fc, double *tru)

Nonlinear multilevel method.

- VPUBLIC void **Vbuildops** (int *nx, int *ny, int *nz, int *nlev, int *ipkey, int *iinfo, int *ido, int *iz, int *mgprol, int *mgcoar, int *mgsolv, int *mgdisc, int *ipc, double *rpc, double *pc, double *ac, double *cc, double *fc, double *xf, double *yf, double *zf, double *gxcf, double *gycf, double *gzcf, double *a1cf, double *a2cf, double *a3cf, double *ccf, double *fcf, double *tcf)

Build operators, boundary arrays, modify affine vectors ido==0: do only fine level ido==1: do only coarse levels (including second op at coarsest) ido==2: do all levels ido==3: rebuild the second operator at the coarsest level.

- VEXTERNC void **Vbuildstr** (int *nx, int *ny, int *nz, int *nlev, int *iz)

Build the nexted operator framework in the array iz.

- VEXTERNC void **Vbuildgaler0** (int *nxf, int *nyf, int *nzf, int *nxc, int *nyc, int *nzc, int *ipkey, int *numdia, double *pcFF, int *ipcFF, double *rpcFF, double *acFF, double *ccFF, double *fcFF, int *ipc, double *rpc, double *ac, double *cc, double *fc)

Form the Galerkin coarse grid system.

- VPUBLIC void **Vxcopy** (int *nx, int *ny, int *nz, double *x, double *y)

A collection of useful low-level routines (timing, etc).

- VEXTERNC void **Vxcopy_small** (int *nx, int *ny, int *nz, double *x, double *y)

Copy operation for a grid function with boundary values. Quite simply copies one 3d matrix to another.

- VEXTERNC void **Vxcopy_large** (int *nx, int *ny, int *nz, double *x, double *y)

Copy operation for a grid function with boundary values. Quite simply copies one 3d matrix to another.

- VEXTERNC void **Vxaxpy** (int *nx, int *ny, int *nz, double *alpha, double *x, double *y)

saxpy operation for a grid function with boundary values.

- VEXTERNC double **Vxnrm1** (int *nx, int *ny, int *nz, double *x)

Norm operation for a grid function with boundary values.

- VEXTERNC double **Vxnrm2** (int *nx, int *ny, int *nz, double *x)

Norm operation for a grid function with boundary values.

- VEXTERNC double **Vxdot** (int *nx, int *ny, int *nz, double *x, double *y)

Inner product operation for a grid function with boundary values.

- VEXTERNC void **Vazeros** (int *nx, int *ny, int *nz, double *x)

Zero out operation for a grid function, including boundary values.

- VEXTERNC void [VfboundPMG](#) (int *ibound, int *nx, int *ny, int *nz, double *x, double *gxc, double *gyc, double *gzc)

Initialize a grid function to have a certain boundary value,.

- VEXTERNC void [VfboundPMG00](#) (int *nx, int *ny, int *nz, double *x)

Initialize a grid function to have a zero boundary value.

- VEXTERNC void [Vaxrand](#) (int *nx, int *ny, int *nz, double *x)

Fill grid function with random values, including boundary values.

- VEXTERNC void [Vxscal](#) (int *nx, int *ny, int *nz, double *fac, double *x)

Scale operation for a grid function with boundary values.

- VEXTERNC void [Vprtmatd](#) (int *nx, int *ny, int *nz, int *ipc, double *rpc, double *ac)
- VPUBLIC void [Vdpbsl](#) (double *abd, int *lda, int *n, int *m, double *b)

LINPACK interface.

- VPUBLIC void [Vmypdefinitpb](#) (int *tnion, double *tcharge, double *tsconc)

Set up the ionic species to be used in later calculations. This must be called before any other of the routines in this file.

- VEXTERNC void [Vmypdefinitnpbe](#) (int *tnion, double *tcharge, double *tsconc)

Set up the ionic species to be used in later calculations. This must be called before any other of the routines in this file.

- VEXTERNC void [Vmypdefinitmpbe](#) (int *tnion, double *tcharge, double *tsconc, double *smvolume, double *smsize)

Set up the ionic species to be used in later calculations. This must be called before any other of the routines in this file.

- VEXTERNC void [Vc_vec](#) (double *coef, double *uin, double *uout, int *nx, int *ny, int *nz, int *ipkey)

Define the nonlinearity (vector version)

- VEXTERNC void [Vdc_vec](#) (double *coef, double *uin, double *uout, int *nx, int *ny, int *nz, int *ipkey)

Define the derivative of the nonlinearity (vector version)

- VEXTERNC void [Vc_vecpmg](#) (double *coef, double *uin, double *uout, int *nx, int *ny, int *nz, int *ipkey)

Define the nonlinearity (vector version)

- VEXTERNC void [Vc_vecsmpbe](#) (double *coef, double *uin, double *uout, int *nx, int *ny, int *nz, int *ipkey)

Define the nonlinearity (vector version)

- VEXTERNC void [Vnewdriv](#) (int *iparm, double *rparm, int *iwork, double *rwork, double *u, double *xf, double *yf, double *zf, double *gxcf, double *gycf, double *gzcf, double *a1cf, double *a2cf, double *a3cf, double *ccf, double *fcf, double *tcf)

Driver for the Newton Solver.

- VEXTERNC void [Vnewdriv2](#) (int *iparm, double *rparm, int *nx, int *ny, int *nz, double *u, int *iz, double *w1, double *w2, int *ipc, double *rpc, double *pc, double *ac, double *cc, double *fc, double *xf, double *yf, double *zf, double *gxcf, double *gycf, double *gzcf, double *a1cf, double *a2cf, double *a3cf, double *ccf, double *fcf, double *tcf)

Solves using Newton's Method.

- VPUBLIC void [Vfnewton](#) (int *nx, int *ny, int *nz, double *x, int *iz, double *w0, double *w1, double *w2, double *w3, int *istop, int *itmax, int *iters, int *ierror, int *nlev, int *ilev, int *nlev_real, int *mgsolv, int *iok, int *iinfo, double *epsiln, double *errtol, double *omega, int *nu1, int *nu2, int *mgsmoo, double *cprime, double *rhs, double *xtmp, int *ipc, double *rpc, double *pc, double *ac, double *cc, double *fc, double *tru)

Driver routines for the Newton method.

- VEXTERNC void [Vnewton](#) (int *nx, int *ny, int *nz, double *x, int *iz, double *w0, double *w1, double *w2, double *w3, int *istop, int *itmax, int *iters, int *ierror, int *nlev, int *ilev, int *nlev_real, int *mgsolv, int *iok, int *iinfo, double *epsiln, double *errtol, double *omega, int *nu1, int *nu2, int *mgsmoo, double *cprime, double *rhs, double *xtmp, int *ipc, double *rpc, double *pc, double *ac, double *cc, double *fc, double *tru)

Inexact-newton-multilevel method.

- VEXTERNC void [Vgetjac](#) (int *nx, int *ny, int *nz, int *nlev_real, int *iz, int *ilev, int *ipkey, double *x, double *r, double *cprime, double *rhs, double *cc, double *pc)

Form the jacobian system.

- VPUBLIC void [Vpower](#) (int *nx, int *ny, int *nz, int *iz, int *ilev, int *ipc, double *rpc, double *ac, double *cc, double *w1, double *w2, double *w3, double *w4, double *eigmax, double *eigmax_model, double *tol, int *itmax, int *iters, int *iinfo)

Power methods for eigenvalue estimation.

- VEXTERN void [Vipower](#) (int *nx, int *ny, int *nz, double *u, int *iz, double *w0, double *w1, double *w2, double *w3, double *w4, double *eigmin, double *eigmin_model, double *tol, int *itmax, int *iters, int *nlev, int *ilev, int *nlev_real, int *mgsolv, int *iok, int *iinfo, double *epsiln, double *errtol, double *omega, int *nu1, int *nu2, int *mgsmoo, int *ipc, double *rpc, double *pc, double *ac, double *cc, double *tru)

Standard inverse power method for minimum eigenvalue estimation.

- VEXTERN void [Vsmooth](#) (int *nx, int *ny, int *nz, int *ipc, double *rpc, double *ac, double *cc, double *fc, double *x, double *w1, double *w2, double *r, int *itmax, int *iters, double *errtol, double *omega, int *iresid, int *iadjoint, int *meth)

Multigrid smoothing functions.

- VEXTERN void [Vnsmooth](#) (int *nx, int *ny, int *nz, int *ipc, double *rpc, double *ac, double *cc, double *fc, double *x, double *w1, double *w2, double *r, int *itmax, int *iters, double *errtol, double *omega, int *iresid, int *iadjoint, int *meth)

call the appropriate non-linear smoothing routine.

7.31.1 Detailed Description

C translation of Holst group PMG code.

7.31.2 Macro Definition Documentation

7.31.2.1 HARMO2

```
#define HARMO2(
    a,
    b ) (2.0 * (a) * (b) / ((a) + (b)))
```

Multigrid subroutines.

Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Version

\$Id:

Attention

```
*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
* Nathan A. Baker (nathan.baker@pnl.gov)
* Pacific Northwest National Laboratory
*
* Additional contributing authors listed in the code documentation.
*
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* PROCUREMENT OF SUBSTITUTE GOODS OR SERVICES; LOSS OF USE, DATA, OR
* PROFITS; OR BUSINESS INTERRUPTION) HOWEVER CAUSED AND ON ANY THEORY OF
* LIABILITY, WHETHER IN CONTRACT, STRICT LIABILITY, OR TORT (INCLUDING
* NEGLIGENCE OR OTHERWISE) ARISING IN ANY WAY OUT OF THE USE OF THIS
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*
*

```

Definition at line 65 of file [mgsubd.h](#).

7.31.2.2 MAXIONS

```
#define MAXIONS 50
```

Specifies the PDE definition for PMG to solve.

Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Version

\$Id:

Attention

```

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*

```

Definition at line 62 of file [mypdec.h](#).

7.31.3 Function Documentation

7.31.3.1 Vaxrand()

```

VEXTERNC void Vaxrand (
    int * nx,
    int * ny,
    int * nz,
    double * x )

```

Fill grid function with random values, including boundary values.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces axrand from mikpckd.f

Parameters

<i>nx</i>	The size of the x dimension of the 3d matrix
<i>ny</i>	The size of the y dimension of the 3d matrix
<i>nz</i>	The size of the z dimension of the 3d matrix
<i>x</i>	The 3d matrix to fill

Definition at line 291 of file [mikpckd.c](#).

7.31.3.2 Vazeros()

```

VEXTERNC void Vazeros (
    int * nx,
    int * ny,
    int * nz,
    double * x )

```

Zero out operation for a grid function, including boundary values.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces azeros from mikpckd.f

Parameters

<i>nx</i>	The size of the x dimension of the 3d matrix
<i>ny</i>	The size of the x dimension of the 3d matrix
<i>nz</i>	The size of the x dimension of the 3d matrix
<i>x</i>	The matrix to zero out

Definition at line 195 of file [mikpckd.c](#).

7.31.3.3 VbuildA()

```

VEXTERNC void VbuildA (
    int * nx,
    int * ny,
    int * nz,
    int * ipkey,
    int * mgdisc,
    int * numdia,
    int * ipc,
    double * rpc,
    double * ac,
    double * cc,
    double * fc,
    double * xf,
    double * yf,
    double * zf,
    double * gxcf,
    double * gycf,
    double * gzcf,
    double * a1cf,
    double * a2cf,
    double * a3cf,
    double * ccf,
    double * fcf )

```

Build the Laplacian.

Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Version

\$Id:

Attention

```

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```

Author

Mike Holst [original], Tucker Beck [translation]

Attention

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```

Break the matrix data-structure into diagonals and then call the matrix build routine

Author

Tucker Beck [C Translation], Michael Holst [Original]

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>ipkey</i>	
<i>mgdisc</i>	
<i>numdia</i>	
<i>ipc</i>	
<i>rpc</i>	
<i>ac</i>	
<i>cc</i>	
<i>fc</i>	
<i>xf</i>	
<i>yf</i>	
<i>zf</i>	
<i>gxcf</i>	
<i>gycf</i>	
<i>gzcf</i>	
<i>a1cf</i>	
<i>a2cf</i>	
<i>a3cf</i>	
<i>ccf</i>	
<i>fcf</i>	

Definition at line 57 of file [buildAd.c](#).

7.31.3.4 Vbuildband()

```
VEXTERNC void Vbuildband (
    int * key,
    int * nx,
    int * ny,
    int * nz,
    int * ipc,
    double * rpc,
    double * ac,
    int * ipcB,
    double * rpcB,
    double * acB )
```

Banded matrix builder.

Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Version

\$Id:

Attention

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* Nathan A. Baker (nathan.baker@pnl.gov)
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```

```
*
*
```

Author

Mike Holst and Steve Bond [original], Tucker Beck [translation]

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```

Build and factor a banded matrix given a matrix in diagonal form.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces buildband from buildBd.f

Parameters

<i>key</i>	
<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>ipc</i>	
<i>rpc</i>	
<i>ac</i>	
<i>ipcB</i>	
<i>rpcB</i>	
<i>acB</i>	

Definition at line 57 of file [buildBd.c](#).

7.31.3.5 Vbuildband1_27()

```

VEXTERNC void Vbuildband1_27 (
    int * nx,
    int * ny,
    int * nz,
    int * ipc,
    double * rpc,
    double * oC,
    double * oE,
    double * oN,
    double * uC,
    double * oNE,
    double * oNW,
    double * uE,
    double * uW,
    double * uN,
    double * uS,
    double * uNE,
    double * uNW,
    double * uSE,
    double * uSW,
    int * ipcB,
    double * rpcB,
    double * acB,
    int * n,
    int * m,
    int * lda )

```

Build the operator in banded form given the 27-diagonal form.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces buildband1_7 from buildBd.f

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>ipc</i>	
<i>rpc</i>	
<i>oC</i>	
<i>oE</i>	
<i>oN</i>	
<i>uC</i>	
<i>oNE</i>	
<i>oNW</i>	
<i>uE</i>	
<i>uW</i>	
<i>uN</i>	
<i>uS</i>	
<i>uNE</i>	
<i>uNW</i>	
<i>uSE</i>	
<i>uSW</i>	
<i>ipcB</i>	
<i>rpcB</i>	
<i>acB</i>	
<i>n</i>	
<i>m</i>	
<i>lda</i>	

Definition at line 183 of file `buildBd.c`.

7.31.3.6 `Vbuildband1_7()`

```

VEXTERNC void Vbuildband1_7 (
    int * nx,
    int * ny,
    int * nz,
    int * ipc,
    double * rpc,
    double * oC,
    double * oE,
    double * oN,
    double * uC,
    int * ipcB,
    double * rpcB,
    double * acB,
    int * n,
    int * m,
    int * lda )

```

Build the operator in banded form given the 7-diagonal form.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces buildband1_7 from buildBd.f

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>ipc</i>	
<i>rpc</i>	
<i>oC</i>	
<i>oE</i>	
<i>oN</i>	
<i>uC</i>	
<i>ipcB</i>	
<i>rpcB</i>	
<i>acB</i>	
<i>n</i>	
<i>m</i>	
<i>lda</i>	

Definition at line 119 of file [buildBd.c](#).

7.31.3.7 VbuildG()

```

VEXTERNC void VbuildG (
    int * nxf,
    int * nyf,
    int * nzf,
    int * nxc,
    int * nyc,
    int * nzc,
    int * numdia,
    double * pcFF,
    double * acFF,
    double * ac )

```

Build Galerkin matrix structures.

Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Version

\$Id:

Attention

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```

Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

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```

Parameters

<i>nx_f</i>	
<i>ny_f</i>	
<i>nz_f</i>	
<i>nx_c</i>	
<i>ny_c</i>	
<i>nz_c</i>	
<i>numdia</i>	
<i>pcFF</i>	
<i>acFF</i>	
<i>ac</i>	

Definition at line 57 of file [buildGd.c](#).

7.31.3.8 VbuildG_1()

```

VEXTERNC void VbuildG_1 (
    int * nxf,
    int * nyf,
    int * nzf,
    int * nx,
    int * ny,
    int * nz,
    double * oPC,
    double * oPN,
    double * oPS,
    double * oPE,
    double * oPW,
    double * oPNE,
    double * oPNW,
    double * oPSE,

```

```

double * oPSW,
double * uPC,
double * uPN,
double * uPS,
double * uPE,
double * uPW,
double * uPNE,
double * uPNW,
double * uPSE,
double * uPSW,
double * dPC,
double * dPN,
double * dPS,
double * dPE,
double * dPW,
double * dPNE,
double * dPNW,
double * dPSE,
double * dPSW,
double * oC,
double * XoC,
double * XoE,
double * XoN,
double * XuC,
double * XoNE,
double * XoNW,
double * XuE,
double * XuW,
double * XuN,
double * XuS,
double * XuNE,
double * XuNW,
double * XuSE,
double * XuSW )

```

Computes a 27-point galerkin coarse grid matrix from a 1-point (i.e., diagonal) fine grid matrix.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces buildG_1 from buildGd.f

Expressions for the galerkin coarse grid stencil XA in terms of the fine grid matrix stencil A and the interpolation operator stencil P. these stencils have the form:

```

XA := array([
matrix([ [ -XdNW(i,j,k), -XdN(i,j,k), -XdNE(i,j,k) ], [ -XdW(i,j,k), -XdC(i,j,k), -XdE(i,j,k) ], [ -XdSW(i,j,k), -XdS(i,j,k), -XdSE(i,j,k) ] ]),
matrix([ [ -XoNW(i,j,k), -XoN(i,j,k), -XoNE(i,j,k) ], [ -XoW(i,j,k), XoC(i,j,k), -XoE(i,j,k) ], [ -XoSW(i,j,k), -XoS(i,j,k), -XoSE(i,j,k) ] ]),
matrix([ [ -XuNW(i,j,k), -XuN(i,j,k), -XuNE(i,j,k) ], [ -XuW(i,j,k), -XuC(i,j,k), -XuE(i,j,k) ], [ -XuSW(i,j,k), -XuS(i,j,k), -XuSE(i,j,k) ] ] ) ):
A := array([
matrix([ [ 0, 0, 0 ], [ 0, 0, 0 ], [ 0, 0, 0 ] ]),
matrix([ [ 0, 0, 0 ], [ 0, oC(i,j,k), 0 ], [ 0, 0, 0 ] ]),

```

```

matrix([ [ 0, 0, 0 ], [ 0, 0, 0 ], [ 0, 0, 0 ]])
P := array([
matrix([ [ dPNW(i,j,k), dPN(i,j,k), dPNE(i,j,k) ], [ dPW(i,j,k), dPC(i,j,k), dPE(i,j,k) ], [ dPSW(i,j,k), dPS(i,j,k), dPSE(i,j,k) ] ]),
matrix([ [ oPNW(i,j,k), oPN(i,j,k), oPNE(i,j,k) ], [ oPW(i,j,k), oPC(i,j,k), oPE(i,j,k) ], [ oPSW(i,j,k), oPS(i,j,k), oPSE(i,j,k) ] ]),
matrix([ [ uPNW(i,j,k), uPN(i,j,k), uPNE(i,j,k) ], [ uPW(i,j,k), uPC(i,j,k), uPE(i,j,k) ], [ uPSW(i,j,k), uPS(i,j,k), uPSE(i,j,k) ] ]))
]:

```

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>oPC</i>	
<i>oPN</i>	
<i>oPS</i>	
<i>oPE</i>	
<i>oPW</i>	
<i>oPNE</i>	
<i>oPNW</i>	
<i>oPSE</i>	
<i>oPSW</i>	
<i>uPC</i>	
<i>uPN</i>	
<i>uPS</i>	
<i>uPE</i>	
<i>uPW</i>	
<i>uPNE</i>	
<i>uPNW</i>	
<i>uPSE</i>	
<i>uPSW</i>	
<i>dPC</i>	
<i>dPN</i>	
<i>dPS</i>	
<i>dPE</i>	
<i>dPW</i>	
<i>dPNE</i>	
<i>dPNW</i>	
<i>dPSE</i>	
<i>dPSW</i>	
<i>oC</i>	
<i>XoC</i>	
<i>XoE</i>	
<i>XoN</i>	
<i>XuC</i>	
<i>XoNE</i>	
<i>XoNW</i>	
<i>XuE</i>	

Parameters

<i>XuW</i>	
<i>XuN</i>	
<i>XuS</i>	
<i>XuNE</i>	
<i>XuNW</i>	
<i>XuSE</i>	
<i>XuSW</i>	

Definition at line 145 of file [buildGd.c](#).

7.31.3.9 VbuildG_27()

```

VEXTERNC void VbuildG_27 (
    int * nxf,
    int * nyf,
    int * nzf,
    int * nx,
    int * ny,
    int * nz,
    double * oPC,
    double * oPN,
    double * oPS,
    double * oPE,
    double * oPW,
    double * oPNE,
    double * oPNW,
    double * oPSE,
    double * oPSW,
    double * uPC,
    double * uPN,
    double * uPS,
    double * uPE,
    double * uPW,
    double * uPNE,
    double * uPNW,
    double * uPSE,
    double * uPSW,
    double * dPC,
    double * dPN,
    double * dPS,
    double * dPE,
    double * dPW,
    double * dPNE,
    double * dPNW,
    double * dPSE,
    double * dPSW,
    double * oC,
    double * oE,
    double * oN,
    double * uC,
    double * oNE,
    double * oNW,

```

```

double * uE,
double * uW,
double * uN,
double * uS,
double * uNE,
double * uNW,
double * uSE,
double * uSW,
double * XoC,
double * XoE,
double * XoN,
double * XuC,
double * XoNE,
double * XoNW,
double * XuE,
double * XuW,
double * XuN,
double * XuS,
double * XuNE,
double * XuNW,
double * XuSE,
double * XuSW )

```

Compute a 27-point galerkin coarse grid matrix from a 27-point fine grid matrix.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces buildG_27 from buildGd.f

Expressions for the galerkin coarse grid stencil XA in terms of the fine grid matrix stencil A and the interpolation operator stencil P. these stencils have the form:

```

XA := array([
matrix([ [ -XdNW(i,j,k), -XdN(i,j,k), -XdNE(i,j,k) ], [ -XdW(i,j,k), -XdC(i,j,k), -XdE(i,j,k) ], [ -XdSW(i,j,k), -XdS(i,j,k), -XdSE(i,j,k) ] ]),
matrix([ [ -XoNW(i,j,k), -XoN(i,j,k), -XoNE(i,j,k) ], [ -XoW(i,j,k), XoC(i,j,k), -XoE(i,j,k) ], [ -XoSW(i,j,k), -XoS(i,j,k), -XoSE(i,j,k) ] ]),
matrix([ [ -XuNW(i,j,k), -XuN(i,j,k), -XuNE(i,j,k) ], [ -XuW(i,j,k), -XuC(i,j,k), -XuE(i,j,k) ], [ -XuSW(i,j,k), -XuS(i,j,k), -XuSE(i,j,k) ] ] ) ]):

```

```

A := array([
matrix([ [ -dNW(i,j,k), -dN(i,j,k), -dNE(i,j,k) ], [ -dW(i,j,k), -dC(i,j,k), -dE(i,j,k) ], [ -dSW(i,j,k), -dS(i,j,k), -dSE(i,j,k) ] ]),
matrix([ [ -oNW(i,j,k), -oN(i,j,k), -oNE(i,j,k) ], [ -oW(i,j,k), oC(i,j,k), -oE(i,j,k) ], [ -oSW(i,j,k), -oS(i,j,k), -oSE(i,j,k) ] ]),
matrix([ [ -uNW(i,j,k), -uN(i,j,k), -uNE(i,j,k) ], [ -uW(i,j,k), -uC(i,j,k), -uE(i,j,k) ], [ -uSW(i,j,k), -uS(i,j,k), -uSE(i,j,k) ] ] ) ]):

```

```

P := array([
matrix([ [ dPNW(i,j,k), dPN(i,j,k), dPNE(i,j,k) ], [ dPW(i,j,k), dPC(i,j,k), dPE(i,j,k) ], [ dPSW(i,j,k), dPS(i,j,k), dPSE(i,j,k) ] ]),
matrix([ [ oPNW(i,j,k), oPN(i,j,k), oPNE(i,j,k) ], [ oPW(i,j,k), oPC(i,j,k), oPE(i,j,k) ], [ oPSW(i,j,k), oPS(i,j,k), oPSE(i,j,k) ] ]),
matrix([ [ uPNW(i,j,k), uPN(i,j,k), uPNE(i,j,k) ], [ uPW(i,j,k), uPC(i,j,k), uPE(i,j,k) ], [ uPSW(i,j,k), uPS(i,j,k), uPSE(i,j,k) ] ] ) ]):

```

in addition, A is assumed to be symmetric so that:

```

oS := proc(x,y,z) RETURN( oN(x,y-1,z) ): end: oW := proc(x,y,z) RETURN( oE(x-1,y,z) ): end: oSE := proc(x,y,z)
RETURN( oNW(x+1,y-1,z) ): end: oSW := proc(x,y,z) RETURN( oNE(x-1,y-1,z) ): end:
dC := proc(x,y,z) RETURN( uC(x,y,z-1) ): end: dW := proc(x,y,z) RETURN( uE(x-1,y,z-1) ): end: dE := proc(x,y,z)
RETURN( uW(x+1,y,z-1) ): end:

```

```

dN := proc(x,y,z) RETURN( uS(x,y+1,z-1) ): end: dNW := proc(x,y,z) RETURN( uSE(x-1,y+1,z-1) ): end: dNE ←
:= proc(x,y,z) RETURN( uSW(x+1,y+1,z-1) ): end:
dS := proc(x,y,z) RETURN( uN(x,y-1,z-1) ): end: dSW := proc(x,y,z) RETURN( uNE(x-1,y-1,z-1) ): end: dSE :=
proc(x,y,z) RETURN( uNW(x+1,y-1,z-1) ): end:

```

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>oPC</i>	
<i>oPN</i>	
<i>oPS</i>	
<i>oPE</i>	
<i>oPW</i>	
<i>oPNE</i>	
<i>oPNW</i>	
<i>oPSE</i>	
<i>oPSW</i>	
<i>uPC</i>	
<i>uPN</i>	
<i>uPS</i>	
<i>uPE</i>	
<i>uPW</i>	
<i>uPNE</i>	
<i>uPNW</i>	
<i>uPSE</i>	
<i>uPSW</i>	
<i>dPC</i>	
<i>dPN</i>	
<i>dPS</i>	
<i>dPE</i>	
<i>dPW</i>	
<i>dPNE</i>	
<i>dPNW</i>	
<i>dPSE</i>	
<i>dPSW</i>	
<i>oC</i>	
<i>oE</i>	
<i>oN</i>	
<i>uC</i>	
<i>oNE</i>	
<i>oNW</i>	
<i>uE</i>	
<i>uW</i>	
<i>uN</i>	
<i>uS</i>	

Parameters

<i>uNE</i>	
<i>uNW</i>	
<i>uSE</i>	
<i>uSW</i>	
<i>XoC</i>	
<i>XoE</i>	
<i>XoN</i>	
<i>XuC</i>	
<i>XoNE</i>	
<i>XoNW</i>	
<i>XuE</i>	
<i>XuW</i>	
<i>XuN</i>	
<i>XuS</i>	
<i>XuNE</i>	
<i>XuNW</i>	
<i>XuSE</i>	
<i>XuSW</i>	

Definition at line 1252 of file [buildGd.c](#).

7.31.3.10 VbuildG_7()

```

VEXTERNC void VbuildG_7 (
    int * nxf,
    int * nyf,
    int * nzf,
    int * nx,
    int * ny,
    int * nz,
    double * oPC,
    double * oPN,
    double * oPS,
    double * oPE,
    double * oPW,
    double * oPNE,
    double * oPNW,
    double * oPSE,
    double * oPSW,
    double * uPC,
    double * uPN,
    double * uPS,
    double * uPE,
    double * uPW,
    double * uPNE,
    double * uPNW,
    double * uPSE,
    double * uPSW,
    double * dPC,
    double * dPN,

```



```

double * dPS,
double * dPE,
double * dPW,
double * dPNE,
double * dPNW,
double * dPSE,
double * dPSW,
double * oC,
double * oE,
double * oN,
double * uC,
double * XoC,
double * XoE,
double * XoN,
double * XuC,
double * XoNE,
double * XoNW,
double * XuE,
double * XuW,
double * XuN,
double * XuS,
double * XuNE,
double * XuNW,
double * XuSE,
double * XuSW )

```

Computes a 27-point galerkin coarse grid matrix from a 7-point fine grid matrix.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces buildG_7 from buildGd.f

Expressions for the galerkin coarse grid stencil XA in terms of the fine grid matrix stencil A and the interpolation operator stencil P. these stencils have the form:

```

XA := array([
matrix([ [ -XdNW(i,j,k), -XdN(i,j,k), -XdNE(i,j,k) ], [ -XdW(i,j,k), -XdC(i,j,k), -XdE(i,j,k) ], [ -XdSW(i,j,k), -XdS(i,j,k), -XdSE(i,j,k) ] ]),
matrix([ [ -XoNW(i,j,k), -XoN(i,j,k), -XoNE(i,j,k) ], [ -XoW(i,j,k), XoC(i,j,k), -XoE(i,j,k) ], [ -XoSW(i,j,k), -XoS(i,j,k), -XoSE(i,j,k) ] ]),
matrix([ [ -XuNW(i,j,k), -XuN(i,j,k), -XuNE(i,j,k) ], [ -XuW(i,j,k), -XuC(i,j,k), -XuE(i,j,k) ], [ -XuSW(i,j,k), -XuS(i,j,k), -XuSE(i,j,k) ] ] )]):
A := array([
matrix([ [ 0, 0, 0 ], [ 0, -dC(i,j,k), 0 ], [ 0, 0, 0 ] ]),
matrix([ [ 0, -oN(i,j,k), 0 ], [ -oW(i,j,k), oC(i,j,k), -oE(i,j,k) ], [ 0, -oS(i,j,k), 0 ] ]),
matrix([ [ 0, 0, 0 ], [ 0, -uC(i,j,k), 0 ], [ 0, 0, 0 ] ] )
P := array([
matrix([ [ dPNW(i,j,k), dPN(i,j,k), dPNE(i,j,k) ], [ dPW(i,j,k), dPC(i,j,k), dPE(i,j,k) ], [ dPSW(i,j,k), dPS(i,j,k), dPSE(i,j,k) ] ]),
matrix([ [ oPNW(i,j,k), oPN(i,j,k), oPNE(i,j,k) ], [ oPW(i,j,k), oPC(i,j,k), oPE(i,j,k) ], [ oPSW(i,j,k), oPS(i,j,k), oPSE(i,j,k) ] ]),
matrix([ [ uPNW(i,j,k), uPN(i,j,k), uPNE(i,j,k) ], [ uPW(i,j,k), uPC(i,j,k), uPE(i,j,k) ], [ uPSW(i,j,k), uPS(i,j,k), uPSE(i,j,k) ] ] )]):

```

in addition, A is assumed to be symmetric so that:

```

oS := proc(x,y,z) RETURN( oN(x,y-1,z) ): end: oW := proc(x,y,z) RETURN( oE(x-1,y,z) ): end: dC := proc(x,y,z) RETURN( uC(x,y,z-1) ): end:

```

Parameters

<i>nx_f</i>	
<i>ny_f</i>	
<i>nz_f</i>	
<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>oPC</i>	
<i>oPN</i>	
<i>oPS</i>	
<i>oPE</i>	
<i>oPW</i>	
<i>oPNE</i>	
<i>oPNW</i>	
<i>oPSE</i>	
<i>oPSW</i>	
<i>uPC</i>	
<i>uPN</i>	
<i>uPS</i>	
<i>uPE</i>	
<i>uPW</i>	
<i>uPNE</i>	
<i>uPNW</i>	
<i>uPSE</i>	
<i>uPSW</i>	
<i>dPC</i>	
<i>dPN</i>	
<i>dPS</i>	
<i>dPE</i>	
<i>dPW</i>	
<i>dPNE</i>	
<i>dPNW</i>	
<i>dPSE</i>	
<i>dPSW</i>	
<i>oC</i>	
<i>oE</i>	
<i>oN</i>	
<i>uC</i>	
<i>XoC</i>	
<i>XoE</i>	
<i>XoN</i>	
<i>XuC</i>	
<i>XoNE</i>	
<i>XoNW</i>	
<i>XuE</i>	
<i>XuW</i>	
<i>XuN</i>	
<i>XuS</i>	

Parameters

<i>XuNE</i>	
<i>XuNW</i>	
<i>XuSE</i>	
<i>XuSW</i>	

Definition at line 450 of file [buildGd.c](#).

7.31.3.11 Vbuildgaler0()

```

VEXTERNC void Vbuildgaler0 (
    int * nxf,
    int * nyf,
    int * nzf,
    int * nxc,
    int * nyc,
    int * nzc,
    int * ipkey,
    int * numdia,
    double * pcFF,
    int * ipcFF,
    double * rpcFF,
    double * acFF,
    double * ccFF,
    double * fcFF,
    int * ipc,
    double * rpc,
    double * ac,
    double * cc,
    double * fc )

```

Form the Galerkin coarse grid system.

Note

Although the fine grid matrix may be 7 or 27 diagonal, the coarse grid matrix is always 27 diagonal. (only 14 stored due to symmetry.)

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces buildgaler0 from mgsbnd.f

Parameters

<i>nxf</i>	
<i>nyf</i>	
<i>nzf</i>	
<i>nxc</i>	
<i>nyc</i>	
<i>nzc</i>	

Parameters

<i>ipkey</i>	
<i>numdia</i>	
<i>pcFF</i>	
<i>ipcFF</i>	
<i>rpcFF</i>	
<i>acFF</i>	
<i>ccFF</i>	
<i>fcFF</i>	
<i>ipc</i>	
<i>rpc</i>	
<i>ac</i>	
<i>cc</i>	
<i>fc</i>	

Definition at line 341 of file [mgsubd.c](#).

7.31.3.12 Vbuildops()

```

VEXTERNC void Vbuildops (
    int * nx,
    int * ny,
    int * nz,
    int * nlev,
    int * ipkey,
    int * iinfo,
    int * ido,
    int * iz,
    int * mgprol,
    int * mgcoar,
    int * mgsolv,
    int * mgdisc,
    int * ipc,
    double * rpc,
    double * pc,
    double * ac,
    double * cc,
    double * fc,
    double * xf,
    double * yf,
    double * zf,
    double * gxcf,
    double * gycf,
    double * gzcf,
    double * alcf,
    double * a2cf,
    double * a3cf,
    double * ccf,
    double * fcf,
    double * tcf )

```

Build operators, boundary arrays, modify affine vectors ido==0: do only fine level ido==1: do only coarse levels (including second op at coarsest) ido==2: do all levels ido==3: rebuild the second operator at the coarsest level.

Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Version

\$Id:

Attention

```
*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
* Nathan A. Baker (nathan.baker@pnl.gov)
* Pacific Northwest National Laboratory
*
* Additional contributing authors listed in the code documentation.
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*
*
```

Note

The fine level must be build before any coarse levels.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Replaces buildops from mgsubd.f

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>nlev</i>	
<i>ipkey</i>	
<i>iinfo</i>	
<i>ido</i>	
<i>iz</i>	
<i>mgprol</i>	
<i>mgcoar</i>	
<i>mgsovl</i>	
<i>mgdisc</i>	
<i>ipc</i>	
<i>rpc</i>	
<i>pc</i>	
<i>ac</i>	
<i>cc</i>	
<i>fc</i>	
<i>xf</i>	
<i>yf</i>	
<i>zf</i>	
<i>gxcf</i>	
<i>gycf</i>	
<i>gzcf</i>	
<i>a1cf</i>	
<i>a2cf</i>	
<i>a3cf</i>	
<i>ccf</i>	
<i>fcf</i>	
<i>tcf</i>	

Definition at line 57 of file [mgsubd.c](#).

7.31.3.13 VbuildP()

```

VEXTERNC void VbuildP (
    int * nxf,
    int * nyf,
    int * nzf,
    int * nxc,
    int * nyc,
    int * nzc,
    int * mgprol,
    int * ipc,
    double * rpc,
    double * pc,
    double * ac,
    double * xf,

```

```
double * yf,
double * zf )
```

Builds prolongation matrix.

Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Version

\$Id:

Attention

```
*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
* Nathan A. Baker (nathan.baker@pnl.gov)
* Pacific Northwest National Laboratory
*
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*
*
```

Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Version**\$Id:****Attention**

```

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* APBS -- Adaptive Poisson-Boltzmann Solver
*
* Nathan A. Baker (nathan.baker@pnl.gov)
* Pacific Northwest National Laboratory
*
* Additional contributing authors listed in the code documentation.
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*
*

```

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>mgprol</i>	
<i>ipc</i>	
<i>rpc</i>	
<i>pc</i>	
<i>ac</i>	
<i>xf</i>	
<i>yf</i>	
<i>zf</i>	

Definition at line 57 of file [buildPd.c](#).

7.31.3.14 Vbuildstr()

```
VEXTERNC void Vbuildstr (
    int * nx,
    int * ny,
    int * nz,
    int * nlev,
    int * iz )
```

Build the nexted operator framework in the array iz.

Note

iz(50,i) indexes into the gridfn arrays for each level i=(1,...,nlev+1) as follows:

```
fun(i) = fun (iz(1,i)) bndx(i) = bndx(iz(2,i)) bndy(i) = bndy(iz(3,i)) bndz(i) = bndz(iz(4,i)) ipc(i) = ipc(iz(5,i)) rpc(i) =
rpc(iz(6,i)) oper(i) = oper(iz(7,i)) grdx(i) = brdx(iz(8,i)) grdy(i) = brdy(iz(9,i)) grdz(i) = brdz(iz(10,i))
```

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces buildstr from mgsubd.f

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>nlev</i>	
<i>iz</i>	

Definition at line 257 of file [mgsubd.c](#).

7.31.3.15 Vc_vec()

```
VEXTERNC void Vc_vec (
    double * coef,
    double * uin,
    double * uout,
    int * nx,
    int * ny,
    int * nz,
    int * ipkey )
```

Define the nonlinearity (vector version)

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces c_vec from mypde.f

Parameters

<i>coef</i>	
<i>uin</i>	
<i>uout</i>	
<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>ipkey</i>	

Definition at line 121 of file [mypdec.c](#).

7.31.3.16 Vc_vecpmg()

```
VEXTERNC void Vc_vecpmg (  
    double * coef,  
    double * uin,  
    double * uout,  
    int * nx,  
    int * ny,  
    int * nz,  
    int * ipkey )
```

Define the nonlinearity (vector version)

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces `c_vecpmg` from `mynde.f`

Parameters

<i>coef</i>	
<i>uin</i>	
<i>uout</i>	
<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>ipkey</i>	

Definition at line 133 of file [mypdec.c](#).

7.31.3.17 Vc_vecsmpbe()

```
VEXTERNC void Vc_vecsmpbe (  
    double * coef,  
    double * uin,  
    double * uout,  
    int * nx,  
    int * ny,  
    int * nz,
```

```
int * ipkey )
```

Define the nonlinearity (vector version)

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces c_vecpmg from mypde.f

Parameters

<i>coef</i>	
<i>uin</i>	
<i>uout</i>	
<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>ipkey</i>	

Definition at line 213 of file [mypdec.c](#).

7.31.3.18 Vcghs()

```

VEXTERNC void Vcghs (
    int * nx,
    int * ny,
    int * nz,
    int * ipc,
    double * rpc,
    double * ac,
    double * cc,
    double * fc,
    double * x,
    double * p,
    double * ap,
    double * r,
    int * itmax,
    int * iters,
    double * errtol,
    double * omega,
    int * iresid,
    int * iadjoint )

```

A collection of useful low-level routines (timing, etc).

Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Version

\$Id:

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Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Version

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```

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>ipc</i>	
<i>rpc</i>	
<i>ac</i>	
<i>cc</i>	
<i>fc</i>	
<i>x</i>	
<i>p</i>	
<i>ap</i>	
<i>r</i>	
<i>itmax</i>	
<i>iters</i>	
<i>errtol</i>	
<i>omega</i>	
<i>iresid</i>	
<i>iadjoint</i>	

Definition at line 57 of file [cgd.c](#).

7.31.3.19 Vdc_vec()

```

VEXTERNC void Vdc_vec (
    double * coef,
    double * uin,

```

```

double * uout,
int * nx,
int * ny,
int * nz,
int * ipkey )

```

Define the derivative of the nonlinearity (vector version)

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces dc_vec from mypde.f

Parameters

<i>coef</i>	
<i>uin</i>	
<i>uout</i>	
<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>ipkey</i>	

Definition at line 341 of file [mypdec.c](#).

7.31.3.20 Vdpbsl()

```

VEXTERNC void Vdpbsl (
    double * abd,
    int * lda,
    int * n,
    int * m,
    double * b )

```

LINPACK interface.

Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Version

\$Id:

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Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

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```

Solves the double precision symmetric positive definite band system $A \cdot X = B$ using the factors computed by `dpbco` or `dpbfa`

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

A division by zero will occur if the input factor contains a zero on the diagonal. Technically this indicates singularity, but it is usually caused by improper subroutine arguments. It will not occur if the subroutines are called correctly and `info == 0`

Replaces `dpbsl` from `mgsbnd.f`

Parameters

<i>abd</i>	The output from <code>dpbco</code> or <code>dpbfa</code>
<i>lda</i>	The leading dimension of the array <code>abd</code>
<i>n</i>	The order of the matrix <code>a</code>
<i>m</i>	The number of diagonals above the main diagonal
<i>b</i>	The right hand side vector

Definition at line 57 of file `mlinpckd.c`.

7.31.3.21 Vextrac()

```

VEXTERNC void Vextrac (
    int * nxf,
    int * nyf,
    int * nzf,
    int * nxc,
    int * ny,
    int * nzc,
    double * xin,
    double * xout )

```

Simple injection of a fine grid function into coarse grid.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces extrac from matvecd.f

Parameters

<i>nx_f</i>	
<i>ny_f</i>	
<i>nz_f</i>	
<i>nx_c</i>	
<i>ny</i>	
<i>nz_c</i>	
<i>x_{in}</i>	
<i>x_{out}</i>	

Definition at line 1078 of file [matvecd.c](#).

7.31.3.22 VfboundPMG()

```

VEXTERNC void VfboundPMG (
    int * ibound,
    int * nx,
    int * ny,
    int * nz,
    double * x,
    double * gxc,
    double * gyc,
    double * gzc )

```

Initialize a grid function to have a certain boundary value,.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces fboundPMG from mikpckd.f

Parameters

<i>ibound</i>	
<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>x</i>	
<i>gxc</i>	
<i>gyc</i>	
<i>gzc</i>	

Definition at line 209 of file [mikpckd.c](#).

7.31.3.23 VfboundPMG00()

```
VEXTERNC void VfboundPMG00 (
    int * nx,
    int * ny,
    int * nz,
    double * x )
```

Initialize a grid function to have a zero boundary value.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces fboundPMG00 from mikpckd.f

Parameters

<i>nx</i>	The size of the x dimension of the 3d matrix
<i>ny</i>	The size of the y dimension of the 3d matrix
<i>nz</i>	The size of the z dimension of the 3d matrix
<i>x</i>	The 3d matrix to initialize

Definition at line 258 of file [mikpckd.c](#).

7.31.3.24 Vfmvfas()

```
VEXTERNC void Vfmvfas (
    int * nx,
    int * ny,
    int * nz,
    double * x,
    int * iz,
    double * w0,
    double * w1,
    double * w2,
    double * w3,
    double * w4,
    int * istop,
    int * itmax,
    int * iters,
    int * ierror,
    int * nlev,
    int * ilev,
    int * nlev_real,
    int * mgsolv,
    int * iok,
    int * iinfo,
    double * epsiln,
    double * ertol,
    double * omega,
    int * nu1,
    int * nu2,
```

```

int * mgs moo,
int * ipc,
double * rpc,
double * pc,
double * ac,
double * cc,
double * fc,
double * tru )

```

Multigrid nonlinear solve iteration routine.

Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Version

\$Id:

Attention

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Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

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```

Nested iteration for a nonlinear multilevel method. Algorithm: nonlinear multigrid iteration (fas)

this routine is the full multigrid front-end for a multigrid v-cycle solver. in other words, it repeatedly calls the v-cycle multigrid solver on successively finer and finer grids.

Note**Author**

Tucker Beck [C Translation], Michael Holst [Original]

Replaces fmvfas from mgfasd.f

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	

Parameters

<i>x</i>	
<i>iz</i>	
<i>w0</i>	
<i>w1</i>	
<i>w2</i>	
<i>w3</i>	
<i>w4</i>	
<i>istop</i>	
<i>itmax</i>	
<i>iters</i>	
<i>ierror</i>	
<i>nlev</i>	
<i>ilev</i>	
<i>nlev_real</i>	
<i>mgsolv</i>	
<i>iok</i>	
<i>iinfo</i>	
<i>epsiln</i>	
<i>errtol</i>	
<i>omega</i>	
<i>nu1</i>	
<i>nu2</i>	
<i>mgsmoo</i>	
<i>ipc</i>	
<i>rpc</i>	
<i>pc</i>	
<i>ac</i>	
<i>cc</i>	
<i>fc</i>	
<i>tru</i>	

Definition at line 57 of file [mgfasd.c](#).

7.31.3.25 Vfnewton()

```

VPUBLIC void Vfnewton (
    int * nx,
    int * ny,
    int * nz,
    double * x,
    int * iz,
    double * w0,
    double * w1,
    double * w2,
    double * w3,
    int * istop,
    int * itmax,
    int * iters,
    int * ierror,

```

```

int * nlev,
int * ilev,
int * nlev_real,
int * mgsolv,
int * iok,
int * iinfo,
double * epsilon,
double * errtol,
double * omega,
int * nul,
int * nu2,
int * mgsmoo,
double * cprime,
double * rhs,
double * xtmp,
int * ipc,
double * rpc,
double * pc,
double * ac,
double * cc,
double * fc,
double * tru )

```

Driver routines for the Newton method.

Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Version

\$Id:

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Nested iteration for an inexact-newton-multilevel method.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces `fnewton` from `newtond.f`

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>x</i>	
<i>iz</i>	
<i>w0</i>	
<i>w1</i>	
<i>w2</i>	
<i>w3</i>	
<i>istop</i>	
<i>itmax</i>	
<i>iters</i>	
<i>ierror</i>	
<i>nlev</i>	
<i>ilev</i>	
<i>nlev_real</i>	
<i>mgsolv</i>	
<i>iok</i>	
<i>iinfo</i>	
<i>epsiln</i>	
<i>errtol</i>	
<i>omega</i>	
<i>nu1</i>	
<i>nu2</i>	
<i>mgsmoo</i>	
<i>cprime</i>	
<i>rhs</i>	
<i>xtmp</i>	
<i>ipc</i>	
<i>rpc</i>	
<i>pc</i>	
<i>ac</i>	
<i>cc</i>	
<i>fc</i>	
<i>tru</i>	

Definition at line 58 of file `newtond.c`.

7.31.3.26 Vgetjac()

```

VEXTERNC void Vgetjac (
    int * nx,
    int * ny,
    int * nz,
    int * nlev_real,
    int * iz,
    int * lev,
    int * ipkey,
    double * x,
    double * r,
    double * cprime,
    double * rhs,
    double * cc,
    double * pc )

```

Form the jacobian system.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces getjac from newtond.f

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>nlev_real</i>	
<i>iz</i>	
<i>lev</i>	
<i>ipkey</i>	
<i>x</i>	
<i>r</i>	
<i>cprime</i>	
<i>rhs</i>	
<i>cc</i>	
<i>pc</i>	

Definition at line 550 of file [newtond.c](#).

7.31.3.27 Vgsrb()

```

VEXTERNC void Vgsrb (
    int * nx,
    int * ny,
    int * nz,
    int * ipc,
    double * rpc,
    double * ac,
    double * cc,

```

```

double * fc,
double * x,
double * w1,
double * w2,
double * r,
int * itmax,
int * iters,
double * errtol,
double * omega,
int * iresid,
int * iadjoint )

```

Guass-Seidel solver.

Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Version

\$Id:

Attention

```

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Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

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*
*
```

Call the fast diagonal iterative method.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces gsrB from gsd.f

Parameters

nx	
ny	

Parameters

<i>nz</i>	
<i>ipc</i>	
<i>rpc</i>	
<i>ac</i>	
<i>cc</i>	
<i>fc</i>	
<i>x</i>	
<i>w1</i>	
<i>w2</i>	
<i>r</i>	
<i>itmax</i>	
<i>iters</i>	
<i>errtol</i>	
<i>omega</i>	
<i>iresid</i>	
<i>iadjoint</i>	

Definition at line 57 of file [gsd.c](#).

7.31.3.28 VinterpPMG()

```

VEXTERNC void VinterpPMG (
    int * nxc,
    int * nyc,
    int * nzc,
    int * nxf,
    int * nyf,
    int * nzf,
    double * xin,
    double * xout,
    double * pc )

```

Apply the prolongation operator.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces interpPMG from matvecd.f

Parameters

<i>nxc</i>	
<i>nyc</i>	
<i>nzc</i>	
<i>nxf</i>	
<i>nyf</i>	
<i>nzf</i>	
<i>xin</i>	
<i>xout</i>	
<i>pc</i>	

Definition at line 915 of file [matvecd.c](#).

7.31.3.29 Vipower()

```
VEXTERNC void Vipower (
    int * nx,
    int * ny,
    int * nz,
    double * u,
    int * iz,
    double * w0,
    double * w1,
    double * w2,
    double * w3,
    double * w4,
    double * eigmin,
    double * eigmin_model,
    double * tol,
    int * itmax,
    int * iters,
    int * nlev,
    int * ilev,
    int * nlev_real,
    int * mgsolv,
    int * iok,
    int * iinfo,
    double * epsilon,
    double * errtol,
    double * omega,
    int * nu1,
    int * nu2,
    int * mgsmoo,
    int * ipc,
    double * rpc,
    double * pc,
    double * ac,
    double * cc,
    double * tru )
```

Standard inverse power method for minimum eigenvalue estimation.

Note

To test, note that the 3d laplacean has min/max eigenvalues:

```
lambda_min = 6 - 2*dcos(pi/(nx-1))
              - 2*dcos(pi/(ny-1))
              - 2*dcos(pi/(nz-1))

lambda_max = 6 - 2*dcos((nx-2)*pi/(nx-1))
              - 2*dcos((ny-2)*pi/(ny-1))
              - 2*dcos((nz-2)*pi/(nz-1))
```

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces ipower from powerd.f

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>u</i>	
<i>iz</i>	
<i>w0</i>	
<i>w1</i>	
<i>w2</i>	
<i>w3</i>	
<i>w4</i>	
<i>eigmin</i>	
<i>eigmin_model</i>	
<i>tol</i>	
<i>itmax</i>	
<i>iters</i>	
<i>nlev</i>	
<i>ilev</i>	
<i>nlev_real</i>	
<i>mgstolv</i>	
<i>iok</i>	
<i>iinfo</i>	
<i>epsiln</i>	
<i>errtol</i>	
<i>omega</i>	
<i>nu1</i>	
<i>nu2</i>	
<i>mgsmoo</i>	
<i>ipc</i>	
<i>rpc</i>	
<i>pc</i>	
<i>ac</i>	
<i>cc</i>	
<i>tru</i>	

Definition at line 165 of file [powerd.c](#).

7.31.3.30 Vmatvec()

```

VEXTERNC void Vmatvec (
    int * nx,
    int * ny,
    int * nz,
    int * ipc,
    double * rpc,
    double * ac,

```

```
double * cc,
double * x,
double * y )
```

Matrix-vector multiplication routines.

Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Version

\$Id:

Attention

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Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

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```

Break the matrix data-structure into diagonals and then call the matrix-vector routine.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces matvec from matvecd.f

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>ipc</i>	
<i>rpc</i>	
<i>ac</i>	
<i>cc</i>	
<i>x</i>	
<i>y</i>	

Definition at line 57 of file [matvecd.c](#).

7.31.3.31 Vmgdriv()

```
VEXTERNC void Vmgdriv (
    int * iparm,
    double * rparm,
    int * iwork,
    double * rwork,
    double * u,
    double * xf,
    double * yf,
    double * zf,
    double * gxcf,
    double * gycf,
    double * gzcf,
    double * a1cf,
    double * a2cf,
    double * a3cf,
    double * ccf,
    double * fcf,
    double * tcf )
```

Multilevel solver driver.

Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Version

\$Id:

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```

Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Version

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```

Author

Tucker Beck [C Translation], Michael Holst [Original]

Replaces mgdriv from mgdrvd.f

Parameters

<i>iparm</i>	
<i>rparm</i>	
<i>iwork</i>	
<i>rwork</i>	
<i>u</i>	
<i>xf</i>	
<i>yf</i>	
<i>zf</i>	
<i>gxcf</i>	
<i>gycf</i>	
<i>gzcf</i>	
<i>a1cf</i>	
<i>a2cf</i>	
<i>a3cf</i>	
<i>ccf</i>	
<i>fcf</i>	
<i>tcf</i>	

Definition at line 57 of file [mgdrvd.c](#).

7.31.3.32 Vmgdriv2()

```

VEXTERNC void Vmgdriv2 (
    int * iparm,
    double * rparm,
    int * nx,
    int * ny,
    int * nz,
    double * u,
    int * iz,
    int * ipc,
    double * rpc,
    double * pc,
    double * ac,
    double * cc,
    double * fc,
    double * xf,
    double * yf,
    double * zf,
    double * gxcf,
    double * gycf,
    double * gzcf,
    double * a1cf,
    double * a2cf,
    double * a3cf,

```

```
double * ccf,
double * fcf,
double * tcf )
```

Solves the pde using the multi-grid method.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Replaces mgdriv2 from mgdrvd.f

This routine uses a multigrid method to solve the following three-dimensional, 2nd order elliptic partial differential equation:

```
lu = f, u in omega
u = g, u on boundary of omega
```

where

```
omega = [xmin,xmax]x[ymin,ymax]x[zmin,zmax]
```

the multigrid code requires the operator in the form:

```
- \nabla \cdot (a \nabla u) + c(u) = f
```

with

$a(x,y,z)$, $f(x,y,z)$, scalar functions (possibly discontinuous) on ω . (discontinuities must be along fine grid lines).
boundary function $g(x,y,z)$ is smooth on boundary of ω .

the function $c(u)$ is a possibly nonlinear function of the unknown u , and varies (possibly discontinuously) with the spatial position also.

user inputs:

the user must provide the coefficients of the differential operator, some initial parameter settings in an integer and a real parameter array, and various work arrays.

Parameters

<i>iparm</i>	
<i>rparm</i>	
<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>u</i>	
<i>iz</i>	
<i>ipc</i>	
<i>rpc</i>	
<i>pc</i>	
<i>ac</i>	
<i>cc</i>	
<i>fc</i>	
<i>xf</i>	
<i>yf</i>	
<i>zf</i>	

Parameters

<i>gxcf</i>	
<i>gycf</i>	
<i>gzcf</i>	
<i>a1cf</i>	
<i>a2cf</i>	
<i>a3cf</i>	
<i>ccf</i>	
<i>fcf</i>	
<i>tcf</i>	

Definition at line 190 of file [mgdrv.c](#).

7.31.3.33 Vmgsz()

```

VEXTERNC void Vmgsz (
    int * mgcoar,
    int * mgdisc,
    int * mgsolv,
    int * nx,
    int * ny,
    int * nz,
    int * nlev,
    int * nxc,
    int * nyc,
    int * nzc,
    int * nf,
    int * nc,
    int * narr,
    int * narrc,
    int * n_rpc,
    int * n_iz,
    int * n_ipc,
    int * iretot,
    int * iintot )

```

This routine computes the required sizes of the real and integer work arrays for the multigrid code. these two sizes are a (complicated) function of input parameters.

The work arrays must have been declared in the calling program as:

```

double precision rwork(iretot)
integer          iwork(iintot)

```

where:

```

iretot  = function_of(mgcoar,mgdisc,mgsolv,nx,ny,nz,nlev)
iintot  = function_of(mgcoar,mgdisc,mgsolv,nx,ny,nz,nlev)

mgcoar  = coarsening technique:
          0=standard discretization
          1=averaged coefficient + standard discretization
          2=algebraic galerkin coarsening

mgdisc  = discretization technique:
          0=box method
          1=fem method

```

```

mgsolv  = coarse grid solver:
          0=conjugate gradients
          1=symmetric banded linpack solver

nx,ny,nz = grid dimensions in each direction,
          including boundary points

nlev     = the number of multigrid levels desired for the
          method.

```

other parameters:

```

nf       = number of unknowns on the finest mesh
          = nx * ny * nz

nc       = number of unknowns on the coarsest mesh

narr     = storage for one vector on all the meshes

narrc    = storage for one vector on all the meshes but the finest

```

the work arrays rwork and iwork will be chopped into smaller pieces according to:

```

double precision ac(STORE)          (system operators on all levels)
double precision pc(27*narrc)       (prol. opers for coarse levels)
double precision cc(narr),fc(narr)  (helmholtz term, rhs -- all levels)
double precision rpc(100*(nlev+1))  (real info for all levels)
integer          ipc(100*(nlev+1))  (integer info for all levels)
integer          iz(50,nlev+1),     (pointers into ac,pc,cc,fc,etc.)

```

where STORE depends on the discretization, coarsening, and coarse grid solver:

```

STORE = 4*nf + 4*narrc + NBAND*nc  (mgdisc=box, mgcoar=stan/harm)
       or = 4*nf + 14*narrc + NBAND*nc (mgdisc=box, mgcoar=gal)
       or = 14*nf + 14*narrc + NBAND*nc (mgdisc=fem, mgcoar=stan/harm/gal)

NBAND = 0                               (mgsolv=iterative)
       or = 1+(nxc-2)*(nyc-2)           (mgsolv=7-pt banded linpack)
       or = 1+(nxc-2)*(nyc-2)+(nxc-2)+1 (mgsolv=27-pt banded linpack)

```

Author

Tucker Beck [C Translation], Michael Holst [Original]

Replaces mgsz from mgdrvd.f

Parameters

<i>mgcoar</i>	
<i>mgdisc</i>	
<i>mgsolv</i>	
<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>nlev</i>	
<i>nxc</i>	
<i>nyc</i>	
<i>nzc</i>	
<i>nf</i>	
<i>nc</i>	

Parameters

<i>narr</i>	
<i>narrc</i>	
<i>n_rpc</i>	
<i>n_iz</i>	
<i>n_ipc</i>	
<i>iretot</i>	
<i>iintot</i>	

Definition at line [562](#) of file [mgdrv.c](#).

7.31.3.34 Vmresid()

```
VEXTERNC void Vmresid (
    int * nx,
    int * ny,
    int * nz,
    int * ipc,
    double * rpc,
    double * ac,
    double * cc,
    double * fc,
    double * x,
    double * r )
```

Break the matrix data-structure into diagonals and then call the residual routine.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces mresid from matvecd.f

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>ipc</i>	
<i>rpc</i>	
<i>ac</i>	
<i>cc</i>	
<i>fc</i>	
<i>x</i>	
<i>r</i>	

Definition at line [426](#) of file [matvecd.c](#).

7.31.3.35 Vmvcs()

```
VEXTERNC void Vmvcs (
```

```

int * nx,
int * ny,
int * nz,
double * x,
int * iz,
double * w0,
double * w1,
double * w2,
double * w3,
int * istop,
int * itmax,
int * iters,
int * ierror,
int * nlev,
int * ilev,
int * nlev_real,
int * mgsolv,
int * iok,
int * iinfo,
double * epsilon,
double * errtol,
double * omega,
int * nu1,
int * nu2,
int * mgsmoo,
int * ipc,
double * rpc,
double * pc,
double * ac,
double * cc,
double * fc,
double * tru )

```

MG helper functions.

Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Version

\$Id:

Attention

```

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*
* Nathan A. Baker (nathan.baker@pnl.gov)
* Pacific Northwest National Laboratory
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Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Version

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*
*
```

Screaming linear multilevel method.

algorithm: linear multigrid iteration (cs)

multigrid v-cycle solver.

input: (1) fine and coarse grid discrete linear operators: L_h, L_H (2) fine grid source function: f_h (3) fine grid approximate solution: u_h

output: (1) fine grid improved solution: u_h

the two-grid algorithm is: (1) pre-smooth: $u1_h = \text{smooth}(L_h, f_h, u_h)$ (2) restrict defect: $d_H = r(L_h(u1_h) - f_h)$ (3) solve for correction: $c_H = L_H^{-1}(d_H)$ (4) prolongate and correct: $u2_h = u1_h - p(c_H)$ (5) post-smooth: $u_h = \text{smooth}(L_h, f_h, u2_h)$

(of course, c_H is determined with another two-grid algorithm)

implementation notes: (0) " $u1_h$ " must be kept on each level until " c_H " is computed, and then both are used to compute " $u2_h$ ". (1) " u_h " (and then " $u1_h$ ") on all levels is stored in the " x " array. (2) " d_H " is identically " f_h " for f_h on the next coarser grid. (3) " c_h " is identically " u_h " for u_h on the next coarser grid. (4) " d_H " is stored in the " r " array (must be kept for post-smooth). (5) " f_h " is stored in the " fc " array. (6) " L_h " on all levels is stored in the " ac " array. (7) signs may be reversed; i.e., residual is used in place of the defect in places, etc.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces mvcs from mgcsd.f

New grid size

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>x</i>	
<i>iz</i>	
<i>w0</i>	
<i>w1</i>	
<i>w2</i>	
<i>w3</i>	
<i>istop</i>	
<i>itmax</i>	
<i>iters</i>	
<i>ierror</i>	
<i>nlev</i>	
<i>ilev</i>	

Parameters

<i>nlev_real</i>	
<i>mgssolv</i>	
<i>iok</i>	
<i>iinfo</i>	
<i>epsiln</i>	
<i>errtol</i>	
<i>omega</i>	
<i>nu1</i>	
<i>nu2</i>	
<i>mgsmoo</i>	
<i>ipc</i>	
<i>rpc</i>	
<i>pc</i>	
<i>ac</i>	
<i>cc</i>	
<i>fc</i>	
<i>tru</i>	

Definition at line 57 of file [mgcsd.c](#).

7.31.3.36 Vmvas()

```

VEXTERNC void Vmvas (
    int * nx,
    int * ny,
    int * nz,
    double * x,
    int * iz,
    double * w0,
    double * w1,
    double * w2,
    double * w3,
    double * w4,
    int * istop,
    int * itmax,
    int * iters,
    int * ierror,
    int * nlev,
    int * ilev,
    int * nlev_real,
    int * mgssolv,
    int * iok,
    int * iinfo,
    double * epsiln,
    double * errtol,
    double * omega,
    int * nu1,
    int * nu2,
    int * mgsmoo,
    int * ipc,

```

```

double * rpc,
double * pc,
double * ac,
double * cc,
double * fc,
double * tru )

```

Nonlinear multilevel method.

Note

Replaces mvfas from mgfasd.f

Author

Tucker Beck [C Translation], Michael Holst [Original]

Algorithm: nonlinear multigrid iteration (fas)

multigrid v-cycle solver.

input: (1) fine and coarse grid discrete nonlinear operators: L_h , L_H (2) fine grid source function: f_h (3) fine grid approximate solution: u_h

output: (1) fine grid improved solution: u_h

the two-grid algorithm is: (1) pre-smooth: $u1_h = \text{smooth}(L_h, f_h, u_h)$ (2) restrict defect: $d_H = r(L_h(u1_h) - f_h)$

restrict solution: $u_H = r(u1_h)$ (3) form coarse grid rhs: $f_H = L_H(u_H) - d_H$ solve for correction: $c_H = L_H^{-1}(f_H)$ (4) prolongate and correct: $u2_h = u1_h - p(c_H - u_H)$ (5) post-smooth: $u_h = \text{smooth}(L_h, f_h, u2_h)$

(of course, c_H is determined with another two-grid algorithm)

implementation notes: (0) " $u1_h$ " and " u_H " must be kept on each level until " c_H " is computed, and then all three are used to compute " $u2_h$ ". (1) " u_h " (and then " $u1_h$ ") on all levels is stored in the "x" array. (2) " u_H " on all levels is stored in the "e" array. (3) " c_h " is identically " u_h " for u_h on the next coarser grid. (4) " d_H " is stored in the "r" array. (5) " f_h " and " f_H " are stored in the "fc" array. (6) " L_h " on all levels is stored in the "ac" array. (7) signs may be reversed; i.e., residual is used in place of the defect in places, etc.

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>x</i>	
<i>iz</i>	
<i>w0</i>	
<i>w1</i>	
<i>w2</i>	
<i>w3</i>	
<i>w4</i>	
<i>istop</i>	
<i>itmax</i>	
<i>iters</i>	
<i>ierror</i>	
<i>nlev</i>	
<i>ilev</i>	
<i>nlev_real</i>	
<i>mgsoLv</i>	
<i>iok</i>	
<i>iinfo</i>	
<i>epsiln</i>	

Parameters

<i>errtol</i>	
<i>omega</i>	
<i>nu1</i>	
<i>nu2</i>	
<i>mgsmoo</i>	
<i>ipc</i>	
<i>rpc</i>	
<i>pc</i>	
<i>ac</i>	
<i>cc</i>	
<i>fc</i>	
<i>tru</i>	

Definition at line 157 of file [mgfasd.c](#).

7.31.3.37 Vmypdefinitlpbe()

```

VEXTERNC void Vmypdefinitlpbe (
    int * tnion,
    double * tcharge,
    double * tsconc )

```

Set up the ionic species to be used in later calculations. This must be called before any other of the routines in this file.

Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Version

\$Id:

Attention

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*
*

```

Author

Tucker Beck [C Translation], Nathan Baker [Original]

Note

Replaces mypdefinitlpbe from mypde.f

Parameters

<i>tnion</i>	The number if ionic species
<i>tcharge</i>	The charge in electrons
<i>tsconc</i>	Prefactor for conterion Boltzmann distribution terms. Basically a scaled concentration -(ion concentration/bulkIonicStrength)/2

Definition at line 57 of file [mypdec.c](#).

7.31.3.38 Vmypdefinitnpbe()

```

VEXTERNC void Vmypdefinitnpbe (
    int * tnion,
    double * tcharge,
    double * tsconc )

```

Set up the ionic species to be used in later calculations. This must be called before any other of the routines in this file.

Author

Tucker Beck [C Translation], Nathan Baker [Original]

Note

Replaces mypdefinitnpbe from mypde.f

Parameters

<i>tnion</i>	The number if ionic species
--------------	-----------------------------

Parameters

<i>tcharge</i>	The charge in electrons
<i>tsconc</i>	Prefactor for conterion Boltzmann distribution terms. Basically a scaled concentration -(ion concentration/bulkIonicStrength)/2

Definition at line 75 of file [mypdec.c](#).

7.31.3.39 Vmypdefinitssmpbe()

```

VEXTERNC void Vmypdefinitssmpbe (
    int * tnion,
    double * tcharge,
    double * tsconc,
    double * smvolume,
    double * smsize )

```

Set up the ionic species to be used in later calculations. This must be called before any other of the routines in this file.

Author

Tucker Beck [C Translation], Nathan Baker [Original]

Note

Replaces mypdefinitssmpbe from mypde.f

Parameters

<i>tnion</i>	The number if ionic species
<i>tcharge</i>	The charge in electrons
<i>tsconc</i>	Prefactor for conterion Boltzmann distribution terms. Basically a scaled concentration -(ion concentration/bulkIonicStrength)/2
<i>smvolume</i>	
<i>smsize</i>	

Definition at line 93 of file [mypdec.c](#).

7.31.3.40 Vnewdriv()

```

VEXTERNC void Vnewdriv (
    int * iparm,
    double * rparm,
    int * iwork,
    double * rwork,
    double * u,
    double * xf,
    double * yf,
    double * zf,
    double * gxcf,
    double * gycf,
    double * gzcf,
    double * a1cf,
    double * a2cf,

```

```

double * a3cf,
double * ccf,
double * fcf,
double * tcf )

```

Driver for the Newton Solver.

Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Version

\$Id:

Attention

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```

Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

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```

Driver for a screaming inexact-newton-multilevel solver.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces newdriv from newdrv.f

Parameters

<i>iparm</i>	
<i>rparm</i>	
<i>iwork</i>	
<i>rwork</i>	
<i>u</i>	
<i>xf</i>	

Parameters

<i>yf</i>	
<i>zf</i>	
<i>gxcf</i>	
<i>gycf</i>	
<i>gzcf</i>	
<i>a1cf</i>	
<i>a2cf</i>	
<i>a3cf</i>	
<i>ccf</i>	
<i>fcf</i>	
<i>tcf</i>	

Definition at line 57 of file [newdrvd.c](#).

7.31.3.41 Vnewdriv2()

```

VEXTERNC void Vnewdriv2 (
    int * iparm,
    double * rparm,
    int * nx,
    int * ny,
    int * nz,
    double * u,
    int * iz,
    double * w1,
    double * w2,
    int * ipc,
    double * rpc,
    double * pc,
    double * ac,
    double * cc,
    double * fc,
    double * xf,
    double * yf,
    double * zf,
    double * gxcf,
    double * gycf,
    double * gzcf,
    double * a1cf,
    double * a2cf,
    double * a3cf,
    double * ccf,
    double * fcf,
    double * tcf )

```

Solves using Newton's Method.

Author

Tucker Beck [C Translation], Michael Holst [Original]

This routine uses a newton's method, combined with a linear multigrid iteration, to solve the following three-dimensional, 2nd order elliptic partial differential equation:

```

lu = f, u in omega
u = g, u on boundary of omega

```

where

```

omega = [xmin,xmax]x[ymin,ymax]x[zmin,zmax]

```

the multigrid code requires the operator in the form:

$$-\nabla \cdot (a \nabla u) + c(u) = f$$

with

$a(x,y,z)$, $f(x,y,z)$, scalar functions (possibly discontinuous) on ω . (discontinuities must be along fine grid lines). boundary function $g(x,y,z)$ is smooth on boundary of ω .

the function $c(u)$ is a possibly nonlinear function of the unknown u , and varies (possibly discontinuously) with the spatial position also.

User inputs:

the user must provide the coefficients of the differential operator, some initial parameter settings in an integer and a real parameter array, and various work arrays.

Note

Replaces newdriv2 from newdrvd.f

Parameters

<i>iparm</i>	
<i>rparm</i>	
<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>u</i>	
<i>iz</i>	
<i>w1</i>	
<i>w2</i>	
<i>ipc</i>	
<i>rpc</i>	
<i>pc</i>	
<i>ac</i>	
<i>cc</i>	
<i>fc</i>	
<i>xf</i>	
<i>yf</i>	
<i>zf</i>	
<i>gxcf</i>	
<i>gycf</i>	
<i>gzcf</i>	
<i>a1cf</i>	
<i>a2cf</i>	
<i>a3cf</i>	
<i>ccf</i>	
<i>fcf</i>	
<i>tcf</i>	

Definition at line 169 of file `newdrvd.c`.

7.31.3.42 Vnewton()

```
VEXTERNC void Vnewton (
    int * nx,
    int * ny,
    int * nz,
    double * x,
    int * iz,
    double * w0,
    double * w1,
    double * w2,
    double * w3,
    int * istop,
    int * itmax,
    int * iters,
    int * ierror,
    int * nlev,
    int * ilev,
    int * nlev_real,
    int * mgsolv,
    int * iok,
    int * iinfo,
    double * epsilon,
    double * errtol,
    double * omega,
    int * nu1,
    int * nu2,
    int * mgsmoo,
    double * cprime,
    double * rhs,
    double * xtmp,
    int * ipc,
    double * rpc,
    double * pc,
    double * ac,
    double * cc,
    double * fc,
    double * tru )
```

Inexact-newton-multilevel method.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces newton from newtond.f

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	

Parameters

<i>x</i>	
<i>iz</i>	
<i>w0</i>	
<i>w1</i>	
<i>w2</i>	
<i>w3</i>	
<i>istop</i>	
<i>itmax</i>	
<i>iters</i>	
<i>ierror</i>	
<i>nlev</i>	
<i>ilev</i>	
<i>nlev_real</i>	
<i>mgsolv</i>	
<i>iok</i>	
<i>iinfo</i>	
<i>epsiln</i>	
<i>errtol</i>	
<i>omega</i>	
<i>nu1</i>	
<i>nu2</i>	
<i>mgsmoo</i>	
<i>cprime</i>	
<i>rhs</i>	
<i>xtmp</i>	
<i>ipc</i>	
<i>rpc</i>	
<i>pc</i>	
<i>ac</i>	
<i>cc</i>	
<i>fc</i>	
<i>tru</i>	

Definition at line 162 of file [newtond.c](#).

7.31.3.43 Vnmatvec()

```

VEXTERNC void Vnmatvec (
    int * nx,
    int * ny,
    int * nz,
    int * ipc,
    double * rpc,
    double * ac,
    double * cc,
    double * x,
    double * y,
    double * w1 )

```

Break the matrix data-structure into diagonals and then call the matrix-vector routine.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces nmatvec from matvecd.f

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>ipc</i>	
<i>rpc</i>	
<i>ac</i>	
<i>cc</i>	
<i>x</i>	
<i>y</i>	
<i>w1</i>	

Definition at line 232 of file [matvecd.c](#).

7.31.3.44 Vnmresid()

```
VEXTERNC void Vnmresid (
    int * nx,
    int * ny,
    int * nz,
    int * ipc,
    double * rpc,
    double * ac,
    double * cc,
    double * fc,
    double * x,
    double * r,
    double * w1 )
```

Break the matrix data-structure into diagonals and then call the residual routine.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces nmresid from matvecd.f

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>ipc</i>	
<i>rpc</i>	

Parameters

<i>ac</i>	
<i>cc</i>	
<i>fc</i>	
<i>x</i>	
<i>r</i>	
<i>w1</i>	

Definition at line 598 of file [matvecd.c](#).

7.31.3.45 Vnsmooth()

```

VEXTERNC void Vnsmooth (
    int * nx,
    int * ny,
    int * nz,
    int * ipc,
    double * rpc,
    double * ac,
    double * cc,
    double * fc,
    double * x,
    double * w1,
    double * w2,
    double * r,
    int * itmax,
    int * iters,
    double * errtol,
    double * omega,
    int * iresid,
    int * iadjoint,
    int * meth )

```

call the appropriate non-linear smoothing routine.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces nsmooth from nsmoothd.f

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>ipc</i>	
<i>rpc</i>	
<i>ac</i>	
<i>cc</i>	
<i>fc</i>	
<i>x</i>	

Parameters

<i>w1</i>	
<i>w2</i>	
<i>r</i>	
<i>itmax</i>	
<i>iters</i>	
<i>errtol</i>	
<i>omega</i>	
<i>iresid</i>	
<i>iadjoint</i>	
<i>meth</i>	

Definition at line 98 of file [smoothd.c](#).

7.31.3.46 Vpower()

```

VEXTERNC void Vpower (
    int * nx,
    int * ny,
    int * nz,
    int * iz,
    int * ilev,
    int * ipc,
    double * rpc,
    double * ac,
    double * cc,
    double * w1,
    double * w2,
    double * w3,
    double * w4,
    double * eigmax,
    double * eigmax_model,
    double * tol,
    int * itmax,
    int * iters,
    int * iinfo )

```

Power methods for eigenvalue estimation.

Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Version

\$Id:

Attention

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*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
* Nathan A. Baker (nathan.baker@pnl.gov)
* Pacific Northwest National Laboratory
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Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

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* Nathan A. Baker (nathan.baker@pnl.gov)
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```

Standard power method for maximum eigenvalue estimation of a matrix $c \times c$

Note

To test, note that the 3d laplacean has min/max eigenvalues: $c \times c$ $\lambda_{\min} = 6 - 2\cos(\pi/(nx-1))$ $c \times c$ $\lambda_{\max} = 6 - 2\cos(\pi/(ny-1))$ $c \times c$ $\lambda_{\min} = 6 - 2\cos(\pi/(nz-1))$ $c \times c$ $\lambda_{\max} = 6 - 2\cos(\pi/(nx-2))$ $c \times c$ $\lambda_{\min} = 6 - 2\cos(\pi/(ny-2))$ $c \times c$ $\lambda_{\max} = 6 - 2\cos(\pi/(nz-2))$ $c \times c$

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces power from powerd.f

Vpower is yet untested as a call stack including it hasn't been found

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>iz</i>	
<i>ilev</i>	
<i>ipc</i>	
<i>rpc</i>	
<i>ac</i>	
<i>cc</i>	
<i>w1</i>	
<i>w2</i>	
<i>w3</i>	
<i>w4</i>	
<i>eigmax</i>	
<i>eigmax_model</i>	
<i>tol</i>	
<i>itmax</i>	
<i>iters</i>	
<i>iinfo</i>	

Definition at line 57 of file [powerd.c](#).

7.31.3.47 Vprtmatd()

```
VEXTERNC void Vprtmatd (
    int * nx,
    int * ny,
    int * nz,
    int * ipc,
    double * rpc,
    double * ac )
```

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces prtmatd from mikpckd.f

Parameters

<i>nx</i>	The size of the x dimension of the 3d matrix
<i>ny</i>	The size of the y dimension of the 3d matrix
<i>nz</i>	The size of the z dimension of the 3d matrix
<i>ipc</i>	Integer parameters
<i>rpc</i>	Double parameters
<i>ac</i>	

Definition at line 332 of file [mikpckd.c](#).

7.31.3.48 Vrestrc()

```
VEXTERNC void Vrestrc (
    int * nxf,
    int * nyf,
    int * nzf,
    int * nxc,
    int * nyc,
    int * nzc,
    double * xin,
    double * xout,
    double * pc )
```

Apply the restriction operator.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces restrc from matvecd.f

Parameters

<i>nx_f</i>	
<i>ny_f</i>	
<i>nz_f</i>	
<i>nx_c</i>	
<i>ny_c</i>	
<i>nz_c</i>	
<i>x_{in}</i>	
<i>x_{out}</i>	
<i>pc</i>	

Definition at line 782 of file [matvecd.c](#).

7.31.3.49 Vsmooth()

```

VEXTERNC void Vsmooth (
    int * nx,
    int * ny,
    int * nz,
    int * ipc,
    double * rpc,
    double * ac,
    double * cc,
    double * fc,
    double * x,
    double * w1,
    double * w2,
    double * r,
    int * itmax,
    int * iters,
    double * errtol,
    double * omega,
    int * iresid,
    int * iadjoint,
    int * meth )

```

Multigrid smoothing functions.

Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Version

\$Id:

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* Nathan A. Baker (nathan.baker@pnl.gov)
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Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

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```

call the appropriate linear smoothing routine.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces smooth from smoothd.f

Parameters

<i>nx</i>	
<i>ny</i>	
<i>nz</i>	
<i>ipc</i>	
<i>rpc</i>	
<i>ac</i>	
<i>cc</i>	
<i>fc</i>	
<i>x</i>	
<i>w1</i>	
<i>w2</i>	
<i>r</i>	
<i>itmax</i>	
<i>iters</i>	
<i>errtol</i>	
<i>omega</i>	
<i>iresid</i>	
<i>iadjoint</i>	
<i>meth</i>	

Definition at line 58 of file [smoothd.c](#).

7.31.3.50 Vxaxpy()

```

VEXTERNC void Vxaxpy (
    int * nx,
    int * ny,
```

```

    int * nz,
    double * alpha,
    double * x,
    double * y )

```

saxpy operation for a grid function with boundary values.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces saxpy from mikpckd.f

Parameters

<i>nx</i>	The size of the x dimension of the 3d matrix
<i>ny</i>	The size of the y dimension of the 3d matrix
<i>nz</i>	The size of the z dimension of the 3d matrix
<i>alpha</i>	
<i>x</i>	The source matrix from which to copy data
<i>y</i>	The destination matrix to receive copied data

Definition at line 112 of file [mikpckd.c](#).

7.31.3.51 Vxcopy()

```

VEXTERNC void Vxcopy (
    int * nx,
    int * ny,
    int * nz,
    double * x,
    double * y )

```

A collection of useful low-level routines (timing, etc).

Author

Tucker Beck [fortran ->c translation], Michael Holst [original]

Version

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Author

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Version

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```

Copy operation for a grid function with boundary values. Quite simply copies one 3d matrix to another

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces xcopy from mikpckd.f

Parameters

<i>nx</i>	The size of the x dimension of the 3d matrix
<i>ny</i>	The size of the y dimension of the 3d matrix
<i>nz</i>	The size of the z dimension of the 3d matrix
<i>x</i>	The source matrix from which to copy data
<i>y</i>	The destination matrix to receive copied data

Definition at line 57 of file [mikpckd.c](#).

7.31.3.52 Vxcopy_large()

```

VEXTERNC void Vxcopy_large (
    int * nx,
    int * ny,
    int * nz,
    double * x,
    double * y )

```

Copy operation for a grid function with boundary values. Quite simply copies one 3d matrix to another.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces xcopy_large from mikpckd.f

Note

This function is exactly equivalent to calling xcopy_small with the matrix arguments reversed.

Parameters

<i>nx</i>	The size of the x dimension of the 3d matrix
<i>ny</i>	The size of the y dimension of the 3d matrix
<i>nz</i>	The size of the z dimension of the 3d matrix
<i>x</i>	The source matrix from which to copy data
<i>y</i>	The destination matrix to receive copied data

Definition at line 91 of file [mikpckd.c](#).

7.31.3.53 Vxcopy_small()

```
VEXTERNC void Vxcopy_small (
    int * nx,
    int * ny,
    int * nz,
    double * x,
    double * y )
```

Copy operation for a grid function with boundary values. Quite simply copies one 3d matrix to another.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces xcopy_small from mikpckd.f

Parameters

<i>nx</i>	The size of the x dimension of the 3d matrix
<i>ny</i>	The size of the y dimension of the 3d matrix
<i>nz</i>	The size of the z dimension of the 3d matrix
<i>x</i>	The source matrix from which to copy data
<i>y</i>	The destination matrix to receive copied data

Definition at line 75 of file [mikpckd.c](#).

7.31.3.54 Vxdot()

```
VEXTERNC double Vxdot (
    int * nx,
    int * ny,
    int * nz,
    double * x,
    double * y )
```

Inner product operation for a grid function with boundary values.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces xdot from mikpckd.f

Parameters

<i>nx</i>	The size of the x dimension of the 3d matrix
<i>ny</i>	The size of the y dimension of the 3d matrix
<i>nz</i>	The size of the z dimension of the 3d matrix
<i>x</i>	The first vector
<i>y</i>	The second vector

Definition at line 173 of file [mikpckd.c](#).

7.31.3.55 Vxnrml()

```
VEXTERNC double Vxnrml (
    int * nx,
    int * ny,
    int * nz,
    double * x )
```

Norm operation for a grid function with boundary values.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces xnrml from mikpckd.f

< Accumulates the calculated normal value

Parameters

<i>nx</i>	The size of the x dimension of the 3d matrix
<i>ny</i>	The size of the y dimension of the 3d matrix
<i>nz</i>	The size of the z dimension of the 3d matrix
<i>x</i>	The matrix to normalize

Definition at line 131 of file [mikpckd.c](#).

7.31.3.56 Vxnrml2()

```
VEXTERNC double Vxnrml2 (
    int * nx,
    int * ny,
    int * nz,
    double * x )
```

Norm operation for a grid function with boundary values.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces `xnrm2` from `mikpckd.f`

< Accumulates the calculated normal value

Parameters

<i>nx</i>	The size of the x dimension of the 3d matrix
<i>ny</i>	The size of the y dimension of the 3d matrix
<i>nz</i>	The size of the z dimension of the 3d matrix
<i>x</i>	The matrix to normalize

Definition at line 152 of file [mikpckd.c](#).

7.31.3.57 Vxscal()

```

VEXTERNC void Vxscal (
    int * nx,
    int * ny,
    int * nz,
    double * fac,
    double * x )

```

Scale operation for a grid function with boundary values.

Author

Tucker Beck [C Translation], Michael Holst [Original]

Note

Replaces `xscal` from `mikpckd.f`

Parameters

<i>nx</i>	The size of the x dimension of the 3d matrix
<i>ny</i>	The size of the y dimension of the 3d matrix
<i>nz</i>	The size of the z dimension of the 3d matrix
<i>fac</i>	The scaling factor
<i>x</i>	The 3d matrix to scale

Definition at line 318 of file [mikpckd.c](#).

7.32 High-level front-end routines**Files**

- file [apbs.h](#)
Header file for header dependencies.
- file [main.c](#)
APBS "front end" program using formatted input files.
- file [routines.h](#)
Header file for front end auxiliary routines.

Data Structures

- struct [AtomForce](#)
Structure to hold atomic forces.

Macros

- #define [APBSRC](#) 13
Return code for APBS during failure.

Typedefs

- typedef struct [AtomForce](#) [AtomForce](#)
Define [AtomForce](#) type.

Functions

- int [main](#) (int argc, char **argv)
The main APBS function.
- VPUBLIC Vrc_Codes [initFE](#) (int icalc, [NOsh](#) *nosh, [FEMparm](#) *feparm, [PBEparm](#) *pbeparm, [Vpbe](#) *pbe[[NOSH_MAXCALC](#)], [Valist](#) *alist[[NOSH_MAXMOL](#)], [Vfetk](#) *fetk[[NOSH_MAXCALC](#)])
Initialize FE solver objects.
- VEXTERNC [Vparam](#) * [loadParameter](#) ([NOsh](#) *nosh)
Loads and returns parameter object.
- VEXTERNC int [loadMolecules](#) ([NOsh](#) *nosh, [Vparam](#) *param, [Valist](#) *alist[[NOSH_MAXMOL](#)])
Load the molecules given in NOsh into atom lists.
- VEXTERNC void [killMolecules](#) ([NOsh](#) *nosh, [Valist](#) *alist[[NOSH_MAXMOL](#)])
Destroy the loaded molecules.
- VEXTERNC int [loadDielMaps](#) ([NOsh](#) *nosh, [Vgrid](#) *dielXMap[[NOSH_MAXMOL](#)], [Vgrid](#) *dielYMap[[NOSH_MAXMOL](#)], [Vgrid](#) *dielZMap[[NOSH_MAXMOL](#)])
Load the dielectric maps given in NOsh into grid objects.
- VEXTERNC void [killDielMaps](#) ([NOsh](#) *nosh, [Vgrid](#) *dielXMap[[NOSH_MAXMOL](#)], [Vgrid](#) *dielYMap[[NOSH_MAXMOL](#)], [Vgrid](#) *dielZMap[[NOSH_MAXMOL](#)])
Destroy the loaded dielectric.
- VEXTERNC int [loadKappaMaps](#) ([NOsh](#) *nosh, [Vgrid](#) *kappa[[NOSH_MAXMOL](#)])
Load the kappa maps given in NOsh into grid objects.
- VEXTERNC void [killKappaMaps](#) ([NOsh](#) *nosh, [Vgrid](#) *kappa[[NOSH_MAXMOL](#)])
Destroy the loaded kappa maps.
- VEXTERNC int [loadPotMaps](#) ([NOsh](#) *nosh, [Vgrid](#) *pot[[NOSH_MAXMOL](#)])
Load the potential maps given in NOsh into grid objects.
- VEXTERNC void [killPotMaps](#) ([NOsh](#) *nosh, [Vgrid](#) *pot[[NOSH_MAXMOL](#)])
Destroy the loaded potential maps.
- VEXTERNC int [loadChargeMaps](#) ([NOsh](#) *nosh, [Vgrid](#) *charge[[NOSH_MAXMOL](#)])
Load the charge maps given in NOsh into grid objects.
- VEXTERNC void [killChargeMaps](#) ([NOsh](#) *nosh, [Vgrid](#) *charge[[NOSH_MAXMOL](#)])
Destroy the loaded charge maps.
- VEXTERNC void [printPBE Parm](#) ([PBEparm](#) *pbeparm)
Print out generic PBE params loaded from input.
- VEXTERNC void [printMG Parm](#) ([MGparm](#) *mgparm, double realCenter[3])
Print out MG-specific params loaded from input.

- VEXTERNC int **initMG** (int icalc, **NOsh** *nosh, **MGparm** *mgparm, **PBEparm** *pbeparm, double realCenter[3], **Vpbe** *pbe[NOSH_MAXCALC], **Valist** *alist[NOSH_MAXMOL], **Vgrid** *dielXMap[NOSH_MAXMOL], **Vgrid** *dielYMap[NOSH_MAXMOL], **Vgrid** *dielZMap[NOSH_MAXMOL], **Vgrid** *kappaMap[NOSH_MAXMOL], **Vgrid** *chargeMap[NOSH_MAXMOL], **Vpmgp** *pmgp[NOSH_MAXCALC], **Vpmg** *pmg[NOSH_MAXCALC], **Vgrid** *potMap[NOSH_MAXMOL])
Initialize an MG calculation.
- VEXTERNC void **killMG** (**NOsh** *nosh, **Vpbe** *pbe[NOSH_MAXCALC], **Vpmgp** *pmgp[NOSH_MAXCALC], **Vpmg** *pmg[NOSH_MAXCALC])
Kill structures initialized during an MG calculation.
- VEXTERNC int **solveMG** (**NOsh** *nosh, **Vpmg** *pmg, **MGparm_CalcType** type)
Solve the PBE with MG.
- VEXTERNC int **setPartMG** (**NOsh** *nosh, **MGparm** *mgparm, **Vpmg** *pmg)
Set MG partitions for calculating observables and performing I/O.
- VEXTERNC int **energyMG** (**NOsh** *nosh, int icalc, **Vpmg** *pmg, int *nenergy, double *totEnergy, double *qf←Energy, double *qmEnergy, double *dielEnergy)
Calculate electrostatic energies from MG solution.
- VEXTERNC void **killEnergy** ()
Kill arrays allocated for energies.
- VEXTERNC int **forceMG** (Vmem *mem, **NOsh** *nosh, **PBEparm** *pbeparm, **MGparm** *mgparm, **Vpmg** *pmg, int *nforce, **AtomForce** **atomForce, **Valist** *alist[NOSH_MAXMOL])
Calculate forces from MG solution.
- VEXTERNC void **killForce** (Vmem *mem, **NOsh** *nosh, int nforce[NOSH_MAXCALC], **AtomForce** *atom←Force[NOSH_MAXCALC])
Free memory from MG force calculation.
- VEXTERNC void **storeAtomEnergy** (**Vpmg** *pmg, int icalc, double **atomEnergy, int *nenergy)
Store energy in arrays for future use.
- VEXTERNC int **writedataFlat** (**NOsh** *nosh, Vcom *com, const char *fname, double totEnergy[NOSH_MAXCALC], double qfEnergy[NOSH_MAXCALC], double qmEnergy[NOSH_MAXCALC], double dielEnergy[NOSH_MAXCALC], int nenergy[NOSH_MAXCALC], double *atomEnergy[NOSH_MAXCALC], int nforce[NOSH_MAXCALC], **AtomForce** *atomForce[NOSH_MAXCALC])
Write out information to a flat file.
- VEXTERNC int **writedataXML** (**NOsh** *nosh, Vcom *com, const char *fname, double totEnergy[NOSH_MAXCALC], double qfEnergy[NOSH_MAXCALC], double qmEnergy[NOSH_MAXCALC], double dielEnergy[NOSH_MAXCALC], int nenergy[NOSH_MAXCALC], double *atomEnergy[NOSH_MAXCALC], int nforce[NOSH_MAXCALC], **AtomForce** *atomForce[NOSH_MAXCALC])
Write out information to an XML file.
- VEXTERNC int **writedataMG** (int rank, **NOsh** *nosh, **PBEparm** *pbeparm, **Vpmg** *pmg)
Write out observables from MG calculation to file.
- VEXTERNC int **writematMG** (int rank, **NOsh** *nosh, **PBEparm** *pbeparm, **Vpmg** *pmg)
Write out operator matrix from MG calculation to file.
- VEXTERNC double **returnEnergy** (Vcom *com, **NOsh** *nosh, double totEnergy[NOSH_MAXCALC], int iprint)
Access net local energy.
- VEXTERNC int **printEnergy** (Vcom *com, **NOsh** *nosh, double totEnergy[NOSH_MAXCALC], int iprint)
Combine and pretty-print energy data (deprecated...see printElecEnergy)
- VEXTERNC int **printElecEnergy** (Vcom *com, **NOsh** *nosh, double totEnergy[NOSH_MAXCALC], int iprint)
Combine and pretty-print energy data.
- VEXTERNC int **printApolEnergy** (**NOsh** *nosh, int iprint)
Combine and pretty-print energy data.

- VEXTERNC int `printForce` (Vcom *com, NOsh *nosh, int nforce[NOSH_MAXCALC], AtomForce *atomForce[NOSH_MAXCALC], int i)
Combine and pretty-print force data (deprecated...see printElecForce)
- VEXTERNC int `printElecForce` (Vcom *com, NOsh *nosh, int nforce[NOSH_MAXCALC], AtomForce *atomForce[NOSH_MAXCALC], int i)
Combine and pretty-print force data.
- VEXTERNC int `printApolForce` (Vcom *com, NOsh *nosh, int nforce[NOSH_MAXCALC], AtomForce *atomForce[NOSH_MAXCALC], int i)
Combine and pretty-print force data.
- VEXTERNC void `startVio` ()
Wrapper to start MALOC Vio layer.
- VEXTERNC int `energyAPOL` (APOLparm *apolparm, double sasa, double sav, double atomsasa[], double atomwcaEnergy[], int numatoms)
Calculate non-polar energies.
- VEXTERNC int `forceAPOL` (Vacc *acc, Vmem *mem, APOLparm *apolparm, int *nforce, AtomForce **atomForce, Valist *alist, Vclist *clist)
Calculate non-polar forces.
- VEXTERNC int `initAPOL` (NOsh *nosh, Vmem *mem, Vparam *param, APOLparm *apolparm, int *nforce, AtomForce **atomForce, Valist *alist)
Upperlevel routine to the non-polar energy and force routines.
- VEXTERNC void `printFEPARM` (int icalc, NOsh *nosh, FEMparm *feparm, Vfetk *fetk[NOSH_MAXCALC])
Print out FE-specific params loaded from input.
- VEXTERNC int `energyFE` (NOsh *nosh, int icalc, Vfetk *fetk[NOSH_MAXCALC], int *nenergy, double *totEnergy, double *qfEnergy, double *qmEnergy, double *dielEnergy)
Calculate electrostatic energies from FE solution.
- VEXTERNC void `killFE` (NOsh *nosh, Vpbe *pbe[NOSH_MAXCALC], Vfetk *fetk[NOSH_MAXCALC], Gem *gm[NOSH_MAXMOL])
Kill structures initialized during an FE calculation.
- VEXTERNC int `preRefineFE` (int i, FEMparm *feparm, Vfetk *fetk[NOSH_MAXCALC])
Pre-refine mesh before solve.
- VEXTERNC int `partFE` (int i, NOsh *nosh, FEMparm *feparm, Vfetk *fetk[NOSH_MAXCALC])
Partition mesh (if applicable)
- VEXTERNC int `solveFE` (int i, PBEparm *pbeparm, FEMparm *feparm, Vfetk *fetk[NOSH_MAXCALC])
Solve-estimate-refine.
- VEXTERNC int `postRefineFE` (int icalc, FEMparm *feparm, Vfetk *fetk[NOSH_MAXCALC])
Estimate error, mark mesh, and refine mesh after solve.
- VEXTERNC int `writedataFE` (int rank, NOsh *nosh, PBEparm *pbeparm, Vfetk *fetk)
Write FEM data to files.
- VEXTERNC Vrc_Codes `loadMeshes` (NOsh *nosh, Gem *gm[NOSH_MAXMOL])
Load the meshes given in NOsh into geometry objects.
- VEXTERNC void `killMeshes` (NOsh *nosh, Gem *alist[NOSH_MAXMOL])
Destroy the loaded meshes.

7.32.1 Detailed Description

7.32.2 Macro Definition Documentation

7.32.2.1 APBSRC

```
#define APBSRC 13
```

Return code for APBS during failure.

Definition at line 93 of file `routines.h`.

7.32.3 Typedef Documentation

7.32.3.1 AtomForce

typedef struct [AtomForce](#) [AtomForce](#)

Define [AtomForce](#) type.

Definition at line 111 of file [routines.h](#).

7.32.4 Function Documentation

7.32.4.1 energyAPOL()

```
VEXTERNC int energyAPOL (
    APOLparm * apolparm,
    double sasa,
    double sav,
    double atomsasa[],
    double atomwcaEnergy[],
    int numatoms )
```

Calculate non-polar energies.

Author

David Gohara

Returns

1 if successful, 0 otherwise

Parameters

<i>sasa</i>	APOLparm object
<i>sav</i>	Solvent accessible surface area
<i>atomsasa</i>	Solvent accessible volume
<i>atomwcaEnergy</i>	Array for SASA per atom *
<i>numatoms</i>	Array for WCA energy per atom * Number of atoms (or size of the above arrays) *

Definition at line 4674 of file [routines.c](#).

7.32.4.2 energyFE()

```
VEXTERNC int energyFE (
    NOsh * nosh,
    int icalc,
    Vfetk * fetk[NOSH\_MAXCALC],
    int * nenergy,
    double * totEnergy,
    double * qfEnergy,
    double * qmEnergy,
    double * dielEnergy )
```

Calculate electrostatic energies from FE solution.

Author

Nathan Baker

Parameters

<i>nosh</i>	Object with parsed input file parameters
<i>icalc</i>	Index of calculation
<i>fetk</i>	FE object array
<i>nenergy</i>	Set to number of entries in energy arrays
<i>totEnergy</i>	Set to total energy (in kT)
<i>qfEnergy</i>	Set to charge-potential energy (in kT)
<i>qmEnergy</i>	Set to mobile ion energy (in kT)
<i>dielEnergy</i>	Set to polarization energy (in kT)

Bug "calcenergy 2" does not work

Returns

1 if successful, 0 otherwise

Calculates the electrostatic energies from an FE calculation. < FE-specific parameters

< PBE-specific parameters

If we're not ignoring this particular NOsh object because it has been rendered invalid, call the Vfetk object's energy calculation function. The flag differences specified have to do with setting specific calculation restrictions (see color variable documentation in function code).

Parameters

<i>nosh</i>	Object with parsed input file parameters
<i>icalc</i>	Calculation index
<i>fetk</i>	FE object array
<i>nenergy</i>	Set to number of entries in energy arrays
<i>totEnergy</i>	Set to total energy (in kT)
<i>qfEnergy</i>	Set to charge-potential energy (in kT)
<i>qmEnergy</i>	Set to mobile ion energy (in kT)
<i>dielEnergy</i>	Set to polarization energy (in kT)

Definition at line 4179 of file [routines.c](#).

7.32.4.3 energyMG()

```

VEXTERNC int energyMG (
    NOsh * nosh,
    int icalc,
    Vpmg * pmg,
    int * nenergy,
    double * totEnergy,
    double * qfEnergy,
    double * qmEnergy,
    double * dielEnergy )

```

Calculate electrostatic energies from MG solution.

Author

Nathan Baker

Parameters

<i>nosh</i>	Object with parsed input file parameters
<i>icalc</i>	Index of calculation
<i>pmg</i>	MG object
<i>nenergy</i>	Set to number of entries in energy arrays
<i>totEnergy</i>	Set to total energy (in kT)
<i>qtEnergy</i>	Set to charge-potential energy (in kT)
<i>qmEnergy</i>	Set to mobile ion energy (in kT)
<i>dielEnergy</i>	Set to polarization energy (in kT)

Returns

1 if successful, 0 otherwise

Definition at line 1569 of file [routines.c](#).**7.32.4.4 forceAPOL()**

```

VEXTERNC int forceAPOL (
    Vacc * acc,
    Vmem * mem,
    APOLparm * apolparm,
    int * nforce,
    AtomForce ** atomForce,
    Valist * alist,
    Vclist * clist )

```

Calculate non-polar forces.

Author

David Gohara

Returns

1 if successful, 0 otherwise

Parameters

<i>acc</i>	Accessiblity object
<i>mem</i>	Memory manager
<i>apolparm</i>	Apolar calculation parameter object
<i>nforce</i>	Number of atomic forces to calculate statements for
<i>atomForce</i>	Object for storing atom forces
<i>alist</i>	Atom list
<i>clist</i>	Cell list for accessibility object

Definition at line 4729 of file [routines.c](#).

7.32.4.5 forceMG()

```
VEXTERNC int forceMG (
    Vmem * mem,
    NOsh * nosh,
    PBEparm * pbeparm,
    MGparm * mgparm,
    Vpmg * pmg,
    int * nforce,
    AtomForce ** atomForce,
    Valist * alist[NOSH_MAXMOL] )
```

Calculate forces from MG solution.

Author

Nathan Baker

Parameters

<i>mem</i>	Memory management object
<i>nosh</i>	Parameters from input file
<i>pbeparm</i>	Generic PBE parameters
<i>mgparm</i>	MG-specific parameters
<i>pmg</i>	MG object
<i>nforce</i>	Set to number of forces in arrays
<i>atomForce</i>	List of atom forces
<i>alist</i>	List of atom lists

Returns

1 if successful, 0 otherwise

Definition at line 1636 of file [routines.c](#).

7.32.4.6 initAPOL()

```
VEXTERNC int initAPOL (
    NOsh * nosh,
    Vmem * mem,
    Vparam * param,
    APOLparm * apolparm,
    int * nforce,
    AtomForce ** atomForce,
    Valist * alist )
```

Upperlevel routine to the non-polar energy and force routines.

Author

David Gohara

1 if successful, 0 otherwise

Parameters

<i>nosh</i>	Input parameter object
<i>mem</i>	Memory manager
<i>param</i>	Atom parameters
<i>apolparm</i>	Apolar calculation parameters
<i>nforce</i>	Number of force calculations
<i>atomForce</i>	Atom force storage object
<i>alist</i>	Atom list

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7.32.4.7 initFE()

```
VEXTERNC Vrc_Codes initFE (  
    int icalc,  
    NOsh * nosh,  
    FEMparm * feparm,  
    PBEparm * pbeparm,  
    Vpbe * pbe[NOSH_MAXCALC],  
    Valist * alist[NOSH_MAXMOL],  
    Vfetk * fetk[NOSH_MAXCALC] )
```

Initialize FE solver objects.

Author

Nathan Baker

Bug THIS FUNCTION IS HARD-CODED TO SOLVE LRPBE

Author

Nathan Baker

Bug THIS FUNCTION IS HARD-CODED TO SOLVE LRPBE

< Loop counter
< Mesh ID
< Loop counter
< Loop counter
< Molecule ID
<
< I/O socket for reading MCSF mesh data
< Total bytes used by this operation
< High-water memory usage for this operation
< The type of mesh being used (see struct for enum values)
<
<
<
<
< Return codes for function calls (see struct for enum value)
< List of atoms being operated on
< Atom/molecule being operated on

Parameters

<i>icalc</i>	Index in pb, fetk to initialize (calculation index)
<i>nosh</i>	Master parameter object
<i>feparm</i>	FE-specific parameters
<i>pbeparm</i>	Generic PBE parameters
<i>pbe</i>	Array of PBE objects
<i>alist</i>	Array of atom lists
<i>fetk</i>	Array of finite element objects

Definition at line 3711 of file [routines.c](#).

7.32.4.8 initMG()

```
VEXTERNC int initMG (
    int icalc,
    NOsh * nosh,
    MGparm * mgparm,
    PBEparm * pbeparm,
    double realCenter[3],
    Vpbe * pbe[NOSH_MAXCALC],
    Valist * alist[NOSH_MAXMOL],
    Vgrid * dielXMap[NOSH_MAXMOL],
    Vgrid * dielYMap[NOSH_MAXMOL],
    Vgrid * dielZMap[NOSH_MAXMOL],
    Vgrid * kappaMap[NOSH_MAXMOL],
    Vgrid * chargeMap[NOSH_MAXMOL],
    Vpmgp * pmgp[NOSH_MAXCALC],
    Vpmg * pmg[NOSH_MAXCALC],
    Vgrid * potMap[NOSH_MAXMOL] )
```

Initialize an MG calculation.

Author

Nathan Baker

Returns

1 if succesful, 0 otherwise

Initialize a multigrid calculation.

Parameters

<i>icalc</i>	Index of calculation in pmg/pmpg arrays
<i>nosh</i>	Object with parsed input file parameters
<i>mgparm</i>	Object with MG-specific parameters
<i>pbeparm</i>	Object with generic PBE parameters
<i>realCenter</i>	The actual center of the current mesh
<i>pbe</i>	Array of Vpbe objects (one for each calc)
<i>alist</i>	Array of atom lists
<i>dielXMap</i>	Array of x-shifted dielectric maps
<i>dielYMap</i>	Array of y-shifted dielectric maps
<i>dielZMap</i>	Array of z-shifted dielectric maps
<i>kappaMap</i>	Array of kappa maps
<i>chargeMap</i>	Array of charge maps
<i>pmgp</i>	Array of MG parameter objects (one for each calc)
<i>pmg</i>	Array of MG objects (one for each calc)
<i>potMap</i>	Array of potential maps

Definition at line 1212 of file [routines.c](#).

7.32.4.9 killChargeMaps()

```
VEXTERNC void killChargeMaps (
```

```

    NOsh * nosh,
    Vgrid * charge[NOSH_MAXMOL] )

```

Destroy the loaded charge maps.

Author

Nathan Baker

Parameters

<i>nosh</i>	NOsh object with input file information
<i>charge</i>	List of charge maps

Definition at line 984 of file [routines.c](#).

7.32.4.10 killDielMaps()

```

VEXTERNC void killDielMaps (
    NOsh * nosh,
    Vgrid * dielXMap[NOSH_MAXMOL],
    Vgrid * dielYMap[NOSH_MAXMOL],
    Vgrid * dielZMap[NOSH_MAXMOL] )

```

Destroy the loaded dielectric.

Author

Nathan Baker

Parameters

<i>nosh</i>	NOsh object with input file information
<i>dielXMap</i>	List of x-shifted dielectric maps
<i>dielYMap</i>	List of y-shifted dielectric maps
<i>dielZMap</i>	List of x-shifted dielectric maps

Definition at line 639 of file [routines.c](#).

7.32.4.11 killEnergy()

```

VEXTERNC void killEnergy ( )

```

Kill arrays allocated for energies.

Author

Nathan Baker

Definition at line 1774 of file [routines.c](#).

7.32.4.12 killFE()

```

VEXTERNC void killFE (
    NOsh * nosh,
    Vpbe * pbe[NOSH_MAXCALC],
    Vfetk * fetk[NOSH_MAXCALC],
    Gem * gem[NOSH_MAXMOL] )

```

Kill structures initialized during an FE calculation.

Author

Nathan Baker

Parameters

<i>pbe</i>	Object with parsed input file parameters
<i>fetk</i>	Array of Vpbe objects for each calc
<i>gem</i>	Array of FEtk objects for each calc Array of geometry manager objects for each calc

Definition at line 3683 of file [routines.c](#).

7.32.4.13 killForce()

```

VEXTERNC void killForce (
    Vmem * mem,
    NOsh * nosh,
    int nforce[NOSH_MAXCALC],
    AtomForce * atomForce[NOSH_MAXCALC] )

```

Free memory from MG force calculation.

Author

Nathan Baker

Parameters

<i>mem</i>	Memory management object
<i>nosh</i>	Parameters from input file
<i>nforce</i>	Number of forces in arrays
<i>atomForce</i>	List of atom forces

Definition at line 1782 of file [routines.c](#).

7.32.4.14 killKappaMaps()

```

VEXTERNC void killKappaMaps (
    NOsh * nosh,
    Vgrid * kappa[NOSH_MAXMOL] )

```

Destroy the loaded kappa maps.

Author

Nathan Baker

Parameters

<i>nosh</i>	NOsh object with input file information
<i>kappa</i>	List of kappa maps

Definition at line 776 of file [routines.c](#).

7.32.4.15 killMeshes()

```
VEXTERNC void killMeshes (
    NOsh * nosh,
    Gem * alist[NOSH_MAXMOL] )
```

Destroy the loaded meshes.

Author

Nathan Baker

Parameters

<i>nosh</i>	NOsh object with input file information
<i>alist</i>	Populated list of geometry objects to be destroyed

7.32.4.16 killIMG()

```
VEXTERNC void killMG (
    NOsh * nosh,
    Vpbe * pbe[NOSH_MAXCALC],
    Vpmgp * pmgp[NOSH_MAXCALC],
    Vpmg * pmg[NOSH_MAXCALC] )
```

Kill structures initialized during an MG calculation.

Author

Nathan Baker

Parameters

<i>pbe</i>	Object with parsed input file parameters
<i>pmgp</i>	Array of Vpbe objects for each calc
<i>pmg</i>	Array of MG parameter objects for each calc Array of MG objects for each calc

Definition at line 1461 of file [routines.c](#).

7.32.4.17 killMolecules()

```
VEXTERNC void killMolecules (
    NOsh * nosh,
    Valist * alist[NOSH_MAXMOL] )
```

Destroy the loaded molecules.

Author

Nathan Baker

Parameters

<i>nosh</i>	NOsh object with input file information
<i>alist</i>	List of atom list objects

Definition at line 233 of file [routines.c](#).

7.32.4.18 killPotMaps()

```
VEXTERNC void killPotMaps (
    NOsh * nosh,
    Vgrid * pot[NOSH_MAXMOL] )
```

Destroy the loaded potential maps.

Author

David Gohara

Parameters

<i>nosh</i>	NOsh object with input file information
<i>pot</i>	List of potential maps

Definition at line 865 of file [routines.c](#).

7.32.4.19 loadChargeMaps()

```
VEXTERNC int loadChargeMaps (
    NOsh * nosh,
    Vgrid * map[NOSH_MAXMOL] )
```

Load the charge maps given in NOsh into grid objects.

Author

Nathan Baker

Parameters

<i>nosh</i>	NOsh object with input file information
<i>charge</i>	List of kappa maps

Returns

1 if successful, 0 otherwise

0 on failure, 1 on success

Definition at line 884 of file [routines.c](#).

7.32.4.20 loadDielMaps()

```
VEXTERNC int loadDielMaps (
    NOsh * nosh,
    Vgrid * dielXMap[NOSH_MAXMOL],
    Vgrid * dielYMap[NOSH_MAXMOL],
    Vgrid * dielZMap[NOSH_MAXMOL] )
```

Load the dielectric maps given in NOsh into grid objects.

Author

Nathan Baker

Parameters

<i>nosh</i>	NOsh object with input file information
<i>dielXMap</i>	List of x-shifted dielectric maps
<i>dielYMap</i>	List of y-shifted dielectric maps
<i>dielZMap</i>	List of x-shifted dielectric maps

Returns

1 if successful, 0 otherwise

Loads dielectric map path data into NOsh object

Returns

1 on success, 0 on error

Definition at line 250 of file [routines.c](#).

7.32.4.21 loadKappaMaps()

```
VEXTERNC int loadKappaMaps (
    NOsh * nosh,
    Vgrid * map[NOSH_MAXMOL] )
```

Load the kappa maps given in NOsh into grid objects.

Author

Nathan Baker

Parameters

<i>nosh</i>	NOsh object with input file information
<i>kappa</i>	List of kappa maps

Returns

1 if successful, 0 otherwise

0 on failure, 1 on success

Definition at line 664 of file [routines.c](#).

7.32.4.22 loadMeshes()

```
VEXTERNC Vrc_Codes loadMeshes (
    NOsh * nosh,
    Gem * gm[NOSH_MAXMOL] )
```

Load the meshes given in NOsh into geometry objects.

Author

Nathan Baker

Returns

Error code on success/failure

Parameters

<i>nosh</i>	NOsh object with input file information
<i>gm</i>	List of geometry objects (to be populated)

7.32.4.23 loadMolecules()

```
VEXTERNC int loadMolecules (
    NOsh * nosh,
    Vparam * param,
    Valist * alist[NOSH_MAXMOL] )
```

Load the molecules given in NOsh into atom lists.

Author

Nathan Baker

Returns

1 if successful, 0 otherwise

Parameters

<i>nosh</i>	NOsh object with input file information
<i>param</i>	NULL (if PQR files only) or pointer to parameter object
<i>alist</i>	List of atom list objects (to be populated)

Definition at line 95 of file [routines.c](#).

7.32.4.24 loadParameter()

```
VEXTERNC Vparam * loadParameter (
    NOsh * nosh )
```

Loads and returns parameter object.

Author

Nathan Baker

Returns

Pointer to parameter object or NULL

Parameters

<i>nosh</i>	Pointer to NOsh object with input file information
-------------	--

Definition at line 60 of file [routines.c](#).

7.32.4.25 loadPotMaps()

```
VEXTERNC int loadPotMaps (
    NOsh * nosh,
```

```
Vgrid * map[NOSH_MAXMOL] )
```

Load the potential maps given in NOsh into grid objects.

Author

David Gohara

Parameters

<i>nosh</i>	NOsh object with input file information
<i>pot</i>	List of potential maps

Returns

1 if successful, 0 otherwise

0 on failure, 1 on success

Definition at line 793 of file [routines.c](#).

7.32.4.26 main()

```
int main (
    int argc,
    char ** argv )
```

The main APBS function.

Author

Nathan Baker, Dave Gohara, Todd Dolinsky

Returns

Status code (0 for success)

Parameters

<i>argc</i>	Number of arguments
<i>argv</i>	Argument strings

Definition at line 80 of file [main.c](#).

7.32.4.27 partFE()

```
VEXTERNC int partFE (
    int i,
    NOsh * nosh,
    FEMparm * feparm,
    Vfetk * fetk[NOSH_MAXCALC] )
```

Partition mesh (if applicable)

Author

Nathan Baker

Parameters

<i>i</i>	Calculation index
<i>nosh</i>	Master parameter object
<i>feparm</i>	FE-specific parameters
<i>fetk</i>	Array of FE solver objects

Returns

1 if successful, 0 otherwise

Definition at line [4039](#) of file [routines.c](#).

7.32.4.28 postRefineFE()

```

VEXTERNC int postRefineFE (
    int icalc,
    FEMparm * feparm,
    Vfetk * fetk[NOSH_MAXCALC] )

```

Estimate error, mark mesh, and refine mesh after solve.

Author

Nathan Baker

Parameters

<i>icalc</i>	Calculation index
<i>feparm</i>	FE-specific parameters
<i>fetk</i>	Array of FE solver objects

Returns

1 if successful, 0 otherwise – note that a 0 will likely imply that either the max number of vertices have been met or no vertices were marked for refinement. In either case, this should not be treated as a fatal error.

Estimates the error, marks the mesh, and refines the mesh after solving.

Returns

1 if successful, 0 otherwise – note that a 0 will likely imply that either the max number of vertices have been met or no vertices were marked for refinement. In either case, this should not be treated as a fatal error.

< Number of vertices in the molecular geometry

< Whether vertices are marked for refinement

Parameters

<i>icalc</i>	Calculation index
<i>feparm</i>	FE-specific parameters
<i>fetk</i>	Array of FE solver objects

Definition at line [4239](#) of file [routines.c](#).

7.32.4.29 preRefineFE()

```
VEXTERNC int preRefineFE (
    int i,
    FEMparm * feparm,
    Vfetk * fetk[NOSH_MAXCALC] )
```

Pre-refine mesh before solve.

Author

Nathan Baker

Parameters

<i>i</i>	Calculation index
<i>nosh</i>	Master parameter object
<i>feparm</i>	FE-specific parameters
<i>fetk</i>	Array of FE solver objects

Returns

1 if successful, 0 otherwise

< Number of vertices in the mesh geometry

< Essentially a boolean; indicates whether further refinement is required after running MC's refinement algorithm.

TODO: could this be optimized by moving nverts out of the loop to just above this initial printout? This depends heavily on whether the number of vertices can change during the calculation. - PCE

Definition at line 4046 of file [routines.c](#).

7.32.4.30 printApolEnergy()

```
VEXTERNC int printApolEnergy (
    NOSH * nosh,
    int iprint )
```

Combine and pretty-print energy data.

Author

David Gohara

Returns

1 if successful, 0 otherwise

Parameters

<i>nosh</i>	Parameters from input file
<i>iprint</i>	Index of energy statement to print

Definition at line 2918 of file [routines.c](#).

7.32.4.31 printApolForce()

```
VEXTERNC int printApolForce (
```

```

Vcom * com,
NOSH * nosh,
int nforce[NOSH_MAXCALC],
AtomForce * atomForce[NOSH_MAXCALC],
int i )

```

Combine and pretty-print force data.

Author

David Gohara

Returns

1 if successful, 0 otherwise

Parameters

<i>nosh</i>	Communications object
<i>nforce</i>	Parameters from input file
<i>atomForce</i>	Number of forces calculated
<i>i</i>	Array of force structures Index of force statement to print

Definition at line [3471](#) of file [routines.c](#).

7.32.4.32 printElecEnergy()

```

VEXTERNC int printElecEnergy (
    Vcom * com,
    NOSH * nosh,
    double totEnergy[NOSH_MAXCALC],
    int iprint )

```

Combine and pretty-print energy data.

Author

David Gohara

Returns

1 if successful, 0 otherwise

Parameters

<i>nosh</i>	Communications object
<i>totEnergy</i>	Parameters from input file
<i>iprint</i>	Array of energies from different calculations Index of energy statement to print

Definition at line [2853](#) of file [routines.c](#).

7.32.4.33 printElecForce()

```

VEXTERNC int printElecForce (
    Vcom * com,
    NOSH * nosh,

```



```

    int nforce[NOSH_MAXCALC],
    AtomForce * atomForce[NOSH_MAXCALC],
    int i )

```

Combine and pretty-print force data.

Author

David Gohara

Returns

1 if successful, 0 otherwise

Parameters

<i>nosh</i>	Communications object
<i>nforce</i>	Parameters from input file
<i>atomForce</i>	Number of forces calculated
<i>i</i>	Array of force structures Index of force statement to print

Definition at line 3228 of file [routines.c](#).

7.32.4.34 printEnergy()

```

VEXTERNC int printEnergy (
    Vcom * com,
    NOsh * nosh,
    double totEnergy[NOSH_MAXCALC],
    int iprint )

```

Combine and pretty-print energy data (deprecated...see printElecEnergy)

Author

Nathan Baker

Returns

1 if successful, 0 otherwise

Parameters

<i>nosh</i>	Communications object
<i>totEnergy</i>	Parameters from input file
<i>iprint</i>	Array of energies from different calculations Index of energy statement to print

Definition at line 2785 of file [routines.c](#).

7.32.4.35 printFEPARM()

```

VEXTERNC void printFEPARM (
    int icalc,
    NOsh * nosh,
    FEMparm * feparm,
    Vfetk * fetk[NOSH_MAXCALC] )

```

Print out FE-specific params loaded from input.

Author

Nathan Baker

Parameters

<i>icalc</i>	Calculation index
<i>nosh</i>	Master parameter object
<i>feparm</i>	FE-specific parameters
<i>fetk</i>	Array of FE solver objects

Definition at line [3903](#) of file [routines.c](#).

7.32.4.36 printForce()

```

VEXTERNC int printForce (
    Vcom * com,
    NOsh * nosh,
    int nforce[NOSH_MAXCALC],
    AtomForce * atomForce[NOSH_MAXCALC],
    int i )

```

Combine and pretty-print force data (deprecated...see printElecForce)

Author

Nathan Baker

Returns

1 if successful, 0 otherwise

Parameters

<i>nosh</i>	Communications object
<i>nforce</i>	Parameters from input file
<i>atomForce</i>	Number of forces calculated
<i>i</i>	Array of force structures Index of force statement to print

Definition at line [2980](#) of file [routines.c](#).

7.32.4.37 printMGPARAM()

```

VEXTERNC void printMGPARAM (
    MGparm * mgparm,
    double realCenter[3] )

```

Print out MG-specific params loaded from input.

Author

Nathan Baker

Parameters

<i>realCenter</i>	Center of mesh for actual calculation
<i>mgparm</i>	MGparm object

Definition at line 1179 of file [routines.c](#).

7.32.4.38 printPBEPARM()

```
VEXTERNC void printPBEPARM (
    PBEparm * pbeparm )
```

Print out generic PBE params loaded from input.

Author

Nathan Baker

Parameters

<i>pbeparm</i>	PBEparm object
----------------	----------------

Definition at line 1002 of file [routines.c](#).

7.32.4.39 returnEnergy()

```
VEXTERNC double returnEnergy (
    Vcom * com,
    NOsh * nosh,
    double totEnergy[NOSH_MAXCALC],
    int iprint )
```

Access net local energy.

Author

Justin Xiang

Parameters

<i>com</i>	Communications object
<i>nosh</i>	Parameters from input file
<i>totEnergy</i>	Array of energies from different calculations
<i>iprint</i>	Index of energy statement to print

Returns

Net local energy

Definition at line 2753 of file [routines.c](#).

7.32.4.40 setPartMG()

```
VEXTERNC int setPartMG (
    NOsh * nosh,
```

```

    MGparm * mgparm,
    Vpmg * pmg )

```

Set MG partitions for calculating observables and performing I/O.

Author

Nathan Baker

Parameters

<i>nosh</i>	Object with parsed input file parameters
<i>mgparm</i>	MG parameters from input file
<i>pmg</i>	MG object

Returns

1 if successful, 0 otherwise

Definition at line 1523 of file [routines.c](#).

7.32.4.41 solveFE()

```

VEXTERNC int solveFE (
    int icalc,
    PBEparm * pbeparm,
    FEMparm * feparm,
    Vfetk * fetk[NOSH_MAXCALC] )

```

Solve-estimate-refine.

Author

Nathan Baker

Parameters

<i>i</i>	Calculation index
<i>feparm</i>	FE-specific parameters
<i>pbeparm</i>	Generic PBE parameters
<i>fetk</i>	Array of FE solver objects

Returns

1 if successful, 0 otherwise

Call MC's mesh solving equations depending upon the type of PBE we're dealing with. < AM_hPcg

< Coarse-grid solver; 0 = SLU, 1 = MG, 2 = CG, 3 = BCG, 4 = PCG, 5 = PBCG

< Primal problem

< Preconditioner; 0 = identity.

Parameters

<i>icalc</i>	Calculation index
<i>pbeparm</i>	PBE-specific parameters
<i>feparm</i>	FE-specific parameters

Parameters

<i>fetk</i>	Array of FE solver objects
-------------	----------------------------

Definition at line 4116 of file [routines.c](#).

7.32.4.42 solveMG()

```
VEXTERNC int solveMG (
    NOsh * nosh,
    Vpmg * pmg,
    MGparm_CalcType type )
```

Solve the PBE with MG.

Author

Nathan Baker

Parameters

<i>nosh</i>	Object with parsed input file parameters
<i>pmg</i>	MG objects for this calculation
<i>type</i>	Type of MG calculation

Returns

1 if successful, 0 otherwise

Definition at line 1487 of file [routines.c](#).

7.32.4.43 startVio()

```
VEXTERNC void startVio ( )
```

Wrapper to start MALOC Vio layer.

Author

Nathan Baker and Robert Konecny

Definition at line 58 of file [routines.c](#).

7.32.4.44 storeAtomEnergy()

```
VEXTERNC void storeAtomEnergy (
    Vpmg * pmg,
    int icalc,
    double ** atomEnergy,
    int * nenergy )
```

Store energy in arrays for future use.

Author

Todd Dolinsky

Parameters

<i>pmg</i>	MG object
<i>icalc</i>	Calculation number
<i>atomEnergy</i>	Pointer to storage array of doubles
<i>nenergy</i>	Stores number of atoms per calc

Definition at line 1870 of file [routines.c](#).

7.32.4.45 writedataFE()

```
VEXTERNC int writedataFE (
    int rank,
    NOsh * nosh,
    PBEparm * pbeparm,
    VFetk * fetk )
```

Write FEM data to files.

Author

Nathan Baker

Parameters

<i>rank</i>	Rank of processor (for parallel runs)
<i>nosh</i>	NOsh object
<i>pbeparm</i>	PBEparm object
<i>fetk</i>	FEtk object (with solution)

Returns

1 if successful, 0 otherwise

Write FEM data to file. <

<

< Loop counter

< Flag indicating whether data can be written to output

<

<

Parameters

<i>rank</i>	Rank of processor (for parallel runs)
<i>nosh</i>	NOsh object
<i>pbeparm</i>	PBE-specific parameters
<i>fetk</i>	FEtk object (with solution)

Definition at line 4300 of file [routines.c](#).

7.32.4.46 writedataFlat()

```
VEXTERNC int writedataFlat (
```

```

    NOsh * nosh,
    Vcom * com,
    const char * fname,
    double totEnergy[NOSH_MAXCALC],
    double qfEnergy[NOSH_MAXCALC],
    double qmEnergy[NOSH_MAXCALC],
    double dielEnergy[NOSH_MAXCALC],
    int nenergy[NOSH_MAXCALC],
    double * atomEnergy[NOSH_MAXCALC],
    int nforce[NOSH_MAXCALC],
    AtomForce * atomForce[NOSH_MAXCALC] )

```

Write out information to a flat file.

Author

Todd Dolinsky

Parameters

<i>nosh</i>	Parameters from input file
<i>com</i>	The communications object
<i>fname</i>	The target XML file name
<i>totEnergy</i>	An array with per-calc total energies (in kT)
<i>qfEnergy</i>	An array with per-calc charge-potential energies (in kT)
<i>qmEnergy</i>	An array with per-calc mobile energies (in kT)
<i>dielEnergy</i>	An array with per-calc polarization energies (in kT)
<i>nenergy</i>	An array containing the number of atoms per-calc
<i>atomEnergy</i>	An array containing per-atom energies (in kT) per calc
<i>nforce</i>	An array containing the number of forces calculated per-calc
<i>atomForce</i>	An array containing per-atom forces per calc

Returns

1 if successful, 0 otherwise

Definition at line 1887 of file [routines.c](#).

7.32.4.47 writedataMG()

```

VEXTERNC int writedataMG (
    int rank,
    NOsh * nosh,
    PBEparm * pbeparm,
    Vpmg * pmg )

```

Write out observables from MG calculation to file.

Author

Nathan Baker

Parameters

<i>rank</i>	Processor rank (if parallel calculation)
-------------	--

Parameters

<i>nosh</i>	Parameters from input file
<i>pbeparm</i>	Generic PBE parameters
<i>pmg</i>	MG object

Returns

1 if successful, 0 otherwise

Definition at line 2383 of file [routines.c](#).

7.32.4.48 writedataXML()

```

VEXTERNC int writedataXML (
    NOsh * nosh,
    Vcom * com,
    const char * fname,
    double totEnergy[NOSH_MAXCALC],
    double qfEnergy[NOSH_MAXCALC],
    double qmEnergy[NOSH_MAXCALC],
    double dielEnergy[NOSH_MAXCALC],
    int nenergy[NOSH_MAXCALC],
    double * atomEnergy[NOSH_MAXCALC],
    int nforce[NOSH_MAXCALC],
    AtomForce * atomForce[NOSH_MAXCALC] )

```

Write out information to an XML file.

Author

Todd Dolinsky

Parameters

<i>nosh</i>	Parameters from input file
<i>com</i>	The communications object
<i>fname</i>	The target XML file name
<i>totEnergy</i>	An array with per-calc total energies (in kT)
<i>qfEnergy</i>	An array with per-calc charge-potential energies (in kT)
<i>qmEnergy</i>	An array with per-calc mobile energies (in kT)
<i>dielEnergy</i>	An array with per-calc polarization energies (in kT)
<i>nenergy</i>	An array containing the number of atoms per-calc
<i>atomEnergy</i>	An array containing per-atom energies (in KT) per calc
<i>nforce</i>	An array containing the number of forces calculated per-calc
<i>atomForce</i>	An array containing per-atom forces per calc

Returns

1 if successful, 0 otherwise

Definition at line 2123 of file [routines.c](#).

7.32.4.49 writematMG()

```
VEEXTERNAL int writematMG (  
    int rank,  
    NOsh * nosh,  
    PBEparm * pbeparm,  
    Vpmg * pmg )
```

Write out operator matrix from MG calculation to file.

Author

Nathan Baker

Parameters

<i>rank</i>	Processor rank (if parallel calculation)
<i>nosh</i>	Parameters from input file
<i>pbeparm</i>	Generic PBE parameters
<i>pmg</i>	MG object

Returns

1 if successful, 0 otherwise

Definition at line 1799 of file [routines.c](#).

Chapter 8

Data Structure Documentation

8.1 AtomForce Struct Reference

Structure to hold atomic forces.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/routines.h>
```

Data Fields

- double [ibForce](#) [3]
- double [qfForce](#) [3]
- double [dbForce](#) [3]
- double [sasaForce](#) [3]
- double [savForce](#) [3]
- double [wcaForce](#) [3]

8.1.1 Detailed Description

Structure to hold atomic forces.

Author

Nathan Baker

Definition at line 99 of file [routines.h](#).

8.1.2 Field Documentation

8.1.2.1 dbForce

```
double dbForce[3]
```

Dielectric boundary force

Definition at line 102 of file [routines.h](#).

8.1.2.2 ibForce

```
double ibForce[3]
```

Ion-boundary force

Definition at line 100 of file [routines.h](#).

8.1.2.3 qfForce

```
double qfForce[3]
```

Charge-field force

Definition at line 101 of file [routines.h](#).

8.1.2.4 sasaForce

```
double sasaForce[3]
```

SASA force (coupled to gamma)

Definition at line 103 of file [routines.h](#).

8.1.2.5 savForce

```
double savForce[3]
```

SAV force (coupled to press)

Definition at line 104 of file [routines.h](#).

8.1.2.6 wcaForce

```
double wcaForce[3]
```

WCA integral force (coupled to bconc)

Definition at line 105 of file [routines.h](#).

The documentation for this struct was generated from the following file:

- [src/routines.h](#)

8.2 sAPOLparm Struct Reference

Parameter structure for APOL-specific variables from input files.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/generic/apolparm.h>
```

Data Fields

- int [parsed](#)
- double [grid](#) [3]
- int [setgrid](#)
- int [molid](#)
- int [setmolid](#)
- double [bconc](#)
- int [setbconc](#)
- double [sdens](#)
- int [setsdens](#)
- double [dpos](#)
- int [setdpos](#)
- double [press](#)
- int [setpress](#)
- Vsurf_Meth [srfm](#)
- int [setsrfm](#)
- double [srad](#)
- int [setsrad](#)
- double [swin](#)
- int [setswin](#)

- double [temp](#)
- int [settemp](#)
- double [gamma](#)
- int [setgamma](#)
- [APOLparm_calcEnergy](#) [calcenergy](#)
- int [setcalcenergy](#)
- [APOLparm_calcForce](#) [calcforce](#)
- int [setcalcforce](#)
- double [watsigma](#)
- double [watepsilon](#)
- double [sasa](#)
- double [sav](#)
- double [wcaEnergy](#)
- double [totForce](#) [3]
- int [setwat](#)

8.2.1 Detailed Description

Parameter structure for APOL-specific variables from input files.

Author

David Gohara

Definition at line [129](#) of file [apolparm.h](#).

8.2.2 Field Documentation

8.2.2.1 bconc

double [bconc](#)

Vacc sphere density

Definition at line [139](#) of file [apolparm.h](#).

8.2.2.2 calcenergy

[APOLparm_calcEnergy](#) [calcenergy](#)

Energy calculation flag

Definition at line [167](#) of file [apolparm.h](#).

8.2.2.3 calcforce

[APOLparm_calcForce](#) [calcforce](#)

Atomic forces calculation

Definition at line [170](#) of file [apolparm.h](#).

8.2.2.4 dpos

double [dpos](#)

Atom position offset

Definition at line [145](#) of file [apolparm.h](#).

8.2.2.5 gamma

double [gamma](#)

Surface tension for apolar energies/forces (in kJ/mol/A²)

Definition at line [163](#) of file [apolparm.h](#).

8.2.2.6 grid

```
double grid[3]
```

Grid spacing

Definition at line 133 of file [apolparm.h](#).

8.2.2.7 molid

```
int molid
```

Molecule ID to perform calculation on

Definition at line 136 of file [apolparm.h](#).

8.2.2.8 parsed

```
int parsed
```

Flag: Has this structure been filled with anything other than the default values? (0 = no, 1 = yes)

Definition at line 131 of file [apolparm.h](#).

8.2.2.9 press

```
double press
```

Solvent pressure

Definition at line 148 of file [apolparm.h](#).

8.2.2.10 sasa

```
double sasa
```

Solvent accessible surface area for this calculation

Definition at line 175 of file [apolparm.h](#).

8.2.2.11 sav

```
double sav
```

Solvent accessible volume for this calculation

Definition at line 176 of file [apolparm.h](#).

8.2.2.12 sdens

```
double sdens
```

Vacc sphere density

Definition at line 142 of file [apolparm.h](#).

8.2.2.13 setbconc

```
int setbconc
```

Flag,

See also

[bconc](#)

Definition at line 140 of file [apolparm.h](#).

8.2.2.14 setcalcenergy

```
int setcalcenergy
```

Flag,

See also

[calcenergy](#)

Definition at line 168 of file [apolparm.h](#).

8.2.2.15 setcalcforce

```
int setcalcforce
```

Flag,

See also

[calcforce](#)

Definition at line 171 of file [apolparm.h](#).

8.2.2.16 setdpos

```
int setdpos
```

Flag,

See also

[dpos](#)

Definition at line 146 of file [apolparm.h](#).

8.2.2.17 setgamma

```
int setgamma
```

Flag,

See also

[gamma](#)

Definition at line 165 of file [apolparm.h](#).

8.2.2.18 setgrid

```
int setgrid
```

Flag,

See also

[grid](#)

Definition at line 134 of file [apolparm.h](#).

8.2.2.19 setmolid

```
int setmolid
```

Flag,

See also

[molid](#)

Definition at line 137 of file [apolparm.h](#).

8.2.2.20 setpress

`int setpress`
Flag,

See also

[press](#)

Definition at line 149 of file [apolparm.h](#).

8.2.2.21 setsdens

`int setsdens`
Flag,

See also

[sdens](#)

Definition at line 143 of file [apolparm.h](#).

8.2.2.22 setsrad

`int setsrad`
Flag,

See also

[srad](#)

Definition at line 155 of file [apolparm.h](#).

8.2.2.23 setsrfm

`int setsrfm`
Flag,

See also

[srfm](#)

Definition at line 152 of file [apolparm.h](#).

8.2.2.24 setswin

`int setswin`
Flag,

See also

[swin](#)

Definition at line 158 of file [apolparm.h](#).

8.2.2.25 settemp

`int settemp`
Flag,

See also

[temp](#)

Definition at line 161 of file [apolparm.h](#).

8.2.2.26 setwat

```
int setwat
```

Boolean for determining if a water parameter is supplied. Yes = 1, No = 0

Definition at line 180 of file [apolparm.h](#).

8.2.2.27 srad

```
double srad
```

Solvent radius

Definition at line 154 of file [apolparm.h](#).

8.2.2.28 srfm

```
Vsurf_Meth srfm
```

Surface calculation method

Definition at line 151 of file [apolparm.h](#).

8.2.2.29 swin

```
double swin
```

Cubic spline window

Definition at line 157 of file [apolparm.h](#).

8.2.2.30 temp

```
double temp
```

Temperature (in K)

Definition at line 160 of file [apolparm.h](#).

8.2.2.31 totForce

```
double totForce[3]
```

Total forces on x, y, z

Definition at line 178 of file [apolparm.h](#).

8.2.2.32 watepsilon

```
double watepsilon
```

Water oxygen Lennard-Jones well depth (kJ/mol)

Definition at line 174 of file [apolparm.h](#).

8.2.2.33 watsigma

```
double watsigma
```

Water oxygen Lennard-Jones radius (A)

Definition at line 173 of file [apolparm.h](#).

8.2.2.34 wcaEnergy

```
double wcaEnergy
```

wcaEnergy

Definition at line 177 of file [apolparm.h](#).

The documentation for this struct was generated from the following file:

- `src/generic/apolparm.h`

8.3 sBEMparm Struct Reference

Parameter structure for BEM-specific variables from input files.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/generic/bemparm.h>
```

Data Fields

- [BEMparm_CalcType](#) type
- int [parsed](#)
- Vchrg_Src [chgs](#)
- int [tree_order](#)
- int [settree_order](#)
- int [tree_n0](#)
- int [settree_n0](#)
- double [mac](#)
- int [setmac](#)
- int [nonlintype](#)
- int [setnonlintype](#)
- int [mesh](#)
- int [setmesh](#)
- int [outdata](#)
- int [setoutdata](#)

8.3.1 Detailed Description

Parameter structure for BEM-specific variables from input files.

Author

Nathan Baker and Todd Dolinsky and Weihua Geng

Note

If you add/delete/change something in this class, the member functions – especially `BEMparm_copy` – must be modified accordingly

Definition at line 96 of file [bemparm.h](#).

8.3.2 Field Documentation

8.3.2.1 chgs

Vchrg_Src [chgs](#)

Charge source (Charge, Multipole, Induced Dipole, NL Induced. Not currently implemented but should be relatively easy to add in the future (cf Pengyu Ren)

Definition at line 102 of file [bemparm.h](#).

8.3.2.2 mac

double [mac](#)

Multipole acceptance criterion (should be between 0 and 1)

Definition at line 108 of file [bemparm.h](#).

8.3.2.3 mesh

`int mesh`

0 for msms, 1 for NanoShaper SES, 2 for NanoShaper Skin

Definition at line 113 of file [bemparm.h](#).

8.3.2.4 nonlintype

`int nonlintype`

Linearity Type Method to be used

Definition at line 110 of file [bemparm.h](#).

8.3.2.5 outdata

`int outdata`

0 does not output vtk, 1 outputs vtk

Definition at line 116 of file [bemparm.h](#).

8.3.2.6 parsed

`int parsed`

Has this structure been filled? (0 = no, 1 = yes)

Definition at line 99 of file [bemparm.h](#).

8.3.2.7 setmac

`int setmac`

Flag,

See also

[mac](#)

Definition at line 109 of file [bemparm.h](#).

8.3.2.8 setmesh

`int setmesh`

Flag,

See also

[mesh](#)

Definition at line 114 of file [bemparm.h](#).

8.3.2.9 setnonlintype

`int setnonlintype`

Flag,

See also

[nonlintype](#)

Definition at line 111 of file [bemparm.h](#).

8.3.2.10 setoutdata

int setoutdata
Flag,

See also

[outdata](#)

Definition at line 117 of file [bemparm.h](#).

8.3.2.11 settree_n0

int settree_n0
Flag,

See also

[tree_npart](#)

Definition at line 107 of file [bemparm.h](#).

8.3.2.12 settree_order

int settree_order
Flag,

See also

[tree_order](#)

Definition at line 105 of file [bemparm.h](#).

8.3.2.13 tree_n0

int tree_n0
Number of particles per leaf of the tree
Definition at line 106 of file [bemparm.h](#).

8.3.2.14 tree_order

int tree_order
User-defined order for the treecode expansion
Definition at line 104 of file [bemparm.h](#).

8.3.2.15 type

[BEMparm_CalcType](#) type
What type of BEM calculation?
Definition at line 98 of file [bemparm.h](#).

The documentation for this struct was generated from the following file:

- [src/generic/bemparm.h](#)

8.4 sFEMparm Struct Reference

Parameter structure for FEM-specific variables from input files.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/generic/femparm.h>
```

Data Fields

- int [parsed](#)
- [FEMparm_CalcType](#) type
- int [settype](#)
- double [glen](#) [3]
- int [setglen](#)
- double [etol](#)
- int [setetol](#)
- [FEMparm_EtolType](#) ekey
- int [setekey](#)
- [FEMparm_EstType](#) akeyPRE
- int [setakeyPRE](#)
- [FEMparm_EstType](#) akeySOLVE
- int [setakeySOLVE](#)
- int [targetNum](#)
- int [settargetNum](#)
- double [targetRes](#)
- int [settargetRes](#)
- int [maxsolve](#)
- int [setmaxsolve](#)
- int [maxvert](#)
- int [setmaxvert](#)
- int [pkey](#)
- int [useMesh](#)
- int [meshID](#)

8.4.1 Detailed Description

Parameter structure for FEM-specific variables from input files.

Author

Nathan Baker

Definition at line 133 of file [femparm.h](#).

8.4.2 Field Documentation

8.4.2.1 akeyPRE

[FEMparm_EstType](#) akeyPRE

Adaptive refinement error estimator method for pre-solution refine. Note, this should either be FRT_UNIF or FRT_GEOM.

Definition at line 148 of file [femparm.h](#).

8.4.2.2 akeySOLVE

[FEMparm_EstType](#) akeySOLVE

Adaptive refinement error estimator method for a posteriori solution-based refinement.

Definition at line 152 of file [femparm.h](#).

8.4.2.3 ekey

`FEMparm_EtolType ekey`

Adaptive refinement interpretation of error tolerance

Definition at line 145 of file [femparm.h](#).

8.4.2.4 etol

`double etol`

Error tolerance for refinement; interpretation depends on the adaptive refinement method chosen

Definition at line 142 of file [femparm.h](#).

8.4.2.5 glen

`double glen[3]`

Domain side lengths (in Å)

Definition at line 140 of file [femparm.h](#).

8.4.2.6 maxsolve

`int maxsolve`

Maximum number of solve-estimate-refine cycles

Definition at line 165 of file [femparm.h](#).

8.4.2.7 maxvert

`int maxvert`

Maximum number of vertices in mesh (ignored if less than zero)

Definition at line 167 of file [femparm.h](#).

8.4.2.8 meshID

`int meshID`

External finite element mesh ID (if used)

Definition at line 174 of file [femparm.h](#).

8.4.2.9 parsed

`int parsed`

Flag: Has this structure been filled with anything other than * the default values? (0 = no, 1 = yes)

Definition at line 135 of file [femparm.h](#).

8.4.2.10 pkey

`int pkey`

Boolean sets the pkey type for going into AM_R refine pkey = 0 for non-HB based methods pkey = 1 for HB based methods

Definition at line 170 of file [femparm.h](#).

8.4.2.11 setakeyPRE

`int setakeyPRE`

Boolean

Definition at line 151 of file [femparm.h](#).

8.4.2.12 setakeySOLVE

```
int setakeySOLVE
```

Boolean

Definition at line 154 of file [femparm.h](#).

8.4.2.13 setekey

```
int setekey
```

Boolean

Definition at line 147 of file [femparm.h](#).

8.4.2.14 setetol

```
int setetol
```

Boolean

Definition at line 144 of file [femparm.h](#).

8.4.2.15 setglen

```
int setglen
```

Boolean

Definition at line 141 of file [femparm.h](#).

8.4.2.16 setmaxsolve

```
int setmaxsolve
```

Boolean

Definition at line 166 of file [femparm.h](#).

8.4.2.17 setmaxvert

```
int setmaxvert
```

Boolean

Definition at line 169 of file [femparm.h](#).

8.4.2.18 settargetNum

```
int settargetNum
```

Boolean

Definition at line 159 of file [femparm.h](#).

8.4.2.19 settargetRes

```
int settargetRes
```

Boolean

Definition at line 164 of file [femparm.h](#).

8.4.2.20 settype

```
int settype
```

Boolean

Definition at line 139 of file [femparm.h](#).

8.4.2.21 targetNum

`int targetNum`

Initial mesh will continue to be marked and refined with the method specified by `akeyPRE` until the mesh contains this many vertices or until `targetRes` is reached.

Definition at line 155 of file [femparm.h](#).

8.4.2.22 targetRes

`double targetRes`

Initial mesh will continue to be marked and refined with the method specified by `akeyPRE` until the mesh contains no markable simplices with longest edges above this size or until `targetNum` is reached.

Definition at line 160 of file [femparm.h](#).

8.4.2.23 type

`FEMparm_CalcType` type

Calculation type

Definition at line 138 of file [femparm.h](#).

8.4.2.24 useMesh

`int useMesh`

Indicates whether we use external finite element mesh

Definition at line 173 of file [femparm.h](#).

The documentation for this struct was generated from the following file:

- [src/generic/femparm.h](#)

8.5 sGEOFLOWparm Struct Reference

Parameter structure for GEOFLOW-specific variables from input files.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/generic/geoflowparm.h>
```

Data Fields

- [GEOFLOWparm_CalcType](#) type
- `int` [parsed](#)
- `int` [vdw](#)
- `int` [setvdw](#)
- `double` [etol](#)

8.5.1 Detailed Description

Parameter structure for GEOFLOW-specific variables from input files.

Author

Andrew Stevens, Kyle Monson

Note

If you add/delete/change something in this class, the member functions – especially `GEOFLOWparm_copy` – must be modified accordingly

Definition at line 98 of file [geoflowparm.h](#).

8.5.2 Field Documentation

8.5.2.1 etol

double etol
user defined error tolerance
Definition at line 106 of file [geoflowparm.h](#).

8.5.2.2 parsed

int parsed
Has this structure been filled? (0 = no, 1 = yes)
Definition at line 101 of file [geoflowparm.h](#).

8.5.2.3 setvdw

int setvdw
Definition at line 105 of file [geoflowparm.h](#).

8.5.2.4 type

[GEOFLOWparm_CalcType](#) type
What type of GEOFLOW calculation?
Definition at line 100 of file [geoflowparm.h](#).

8.5.2.5 vdw

int vdw
Definition at line 104 of file [geoflowparm.h](#).
The documentation for this struct was generated from the following file:

- [src/generic/geoflowparm.h](#)

8.6 sMGparm Struct Reference

Parameter structure for MG-specific variables from input files.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/generic/mgparm.h>
```

Data Fields

- [MGparm_CalcType](#) type
- int [parsed](#)
- int [dime](#) [3]
- int [setdime](#)
- Vchrg_Meth [chgm](#)
- int [setchgm](#)
- Vchrg_Src [chgs](#)
- int [nlev](#)
- int [setnlev](#)
- double [etol](#)
- int [setetol](#)
- double [grid](#) [3]
- int [setgrid](#)
- double [glen](#) [3]

- int [setglen](#)
- [MGparm_CentMeth](#) cmeth
- double [center](#) [3]
- int [centmol](#)
- int [setgcent](#)
- double [cglen](#) [3]
- int [setcglen](#)
- double [fglen](#) [3]
- int [setfglen](#)
- [MGparm_CentMeth](#) ccmeth
- double [ccenter](#) [3]
- int [ccentmol](#)
- int [setcgcent](#)
- [MGparm_CentMeth](#) fcmeth
- double [fcenter](#) [3]
- int [fcentmol](#)
- int [setfgcent](#)
- double [partDisjCenter](#) [3]
- double [partDisjLength](#) [3]
- int [partDisjOwnSide](#) [6]
- int [pdime](#) [3]
- int [setpdime](#)
- int [proc_rank](#)
- int [setrank](#)
- int [proc_size](#)
- int [setsize](#)
- double [ofrac](#)
- int [setofrac](#)
- int [async](#)
- int [setasync](#)
- int [nonlintype](#)
- int [setnonlintype](#)
- int [method](#)
- int [setmethod](#)
- int [useAqua](#)
- int [setUseAqua](#)

8.6.1 Detailed Description

Parameter structure for MG-specific variables from input files.

Author

Nathan Baker and Todd Dolinsky

Note

If you add/delete/change something in this class, the member functions – especially `MGparm_copy` – must be modified accordingly

Definition at line 114 of file [mgparm.h](#).

8.6.2 Field Documentation

8.6.2.1 async

```
int async
```

Processor ID for asynchronous calculation

Definition at line 186 of file [mgparm.h](#).

8.6.2.2 ccenter

```
double ccenter[3]
```

Coarse grid center.

Definition at line 157 of file [mgparm.h](#).

8.6.2.3 ccentmol

```
int ccentmol
```

Particular molecule on which we want to center the grid. This should be the appropriate index in an array of molecules, not the positive definite integer specified by the user.

Definition at line 158 of file [mgparm.h](#).

8.6.2.4 ccmeth

```
MGparm_CentMeth ccmeth
```

Coarse grid centering method

Definition at line 156 of file [mgparm.h](#).

8.6.2.5 center

```
double center[3]
```

Grid center. If ispart = 0, then this is only meaningful if cmeth = 0. However, if ispart = 1 and cmeth = MCM_PNT, then this is the center of the non-disjoint (overlapping) partition. If ispart = 1 and cmeth = MCM_MOL, then this is the vector that must be added to the center of the molecule to give the center of the non-disjoint partition.

Definition at line 138 of file [mgparm.h](#).

8.6.2.6 centmol

```
int centmol
```

Particular molecule on which we want to center the grid. This should be the appropriate index in an array of molecules, not the positive definite integer specified by the user.

Definition at line 146 of file [mgparm.h](#).

8.6.2.7 cglen

```
double cglen[3]
```

Coarse grid side lengths

Definition at line 152 of file [mgparm.h](#).

8.6.2.8 chgm

```
Vchrg_Meth chgm
```

Charge discretization method

Definition at line 122 of file [mgparm.h](#).

8.6.2.9 chgs

`Vchrg_Src chgs`

Charge source (Charge, Multipole, Induced Dipole, NL Induced

Definition at line 124 of file [mgparm.h](#).

8.6.2.10 cmeth

`MGparm_CentMeth cmeth`

Centering method

Definition at line 137 of file [mgparm.h](#).

8.6.2.11 dime

`int dime[3]`

Grid dimensions

Definition at line 120 of file [mgparm.h](#).

8.6.2.12 etol

`double etol`

User-defined error tolerance

Definition at line 131 of file [mgparm.h](#).

8.6.2.13 fcenter

`double fcenter[3]`

Fine grid center.

Definition at line 163 of file [mgparm.h](#).

8.6.2.14 fcentmol

`int fcentmol`

Particular molecule on which we want to center the grid. This should be the appropriate index in an array of molecules, not the positive definite integer specified by the user.

Definition at line 164 of file [mgparm.h](#).

8.6.2.15 fcmeth

`MGparm_CentMeth fcmeth`

Fine grid centering method

Definition at line 162 of file [mgparm.h](#).

8.6.2.16 fglen

`double fglen[3]`

Fine grid side lengths

Definition at line 154 of file [mgparm.h](#).

8.6.2.17 glen

`double glen[3]`

Grid side lengths.

Definition at line 135 of file [mgparm.h](#).

8.6.2.18 grid

```
double grid[3]
```

Grid spacings

Definition at line 133 of file [mgparm.h](#).

8.6.2.19 method

```
int method
```

Solver Method

Definition at line 192 of file [mgparm.h](#).

8.6.2.20 nlev

```
int nlev
```

Levels in multigrid hierarchy

Deprecated Just ignored now

Definition at line 128 of file [mgparm.h](#).

8.6.2.21 nonlotype

```
int nonlotype
```

Linearity Type Method to be used

Definition at line 189 of file [mgparm.h](#).

8.6.2.22 ofrac

```
double ofrac
```

Overlap fraction between procs

Definition at line 184 of file [mgparm.h](#).

8.6.2.23 parsed

```
int parsed
```

Has this structure been filled? (0 = no, 1 = yes)

Definition at line 117 of file [mgparm.h](#).

8.6.2.24 partDisjCenter

```
double partDisjCenter[3]
```

This gives the center of the disjoint partitions

Definition at line 171 of file [mgparm.h](#).

8.6.2.25 partDisjLength

```
double partDisjLength[3]
```

This gives the lengths of the disjoint partitions

Definition at line 173 of file [mgparm.h](#).

8.6.2.26 partDisjOwnSide

```
int partDisjOwnSide[6]
```

Tells whether the boundary points are ours (1) or not (0)

Definition at line 175 of file [mgparm.h](#).

8.6.2.27 pdime

```
int pdime[3]
```

Grid of processors to be used in calculation

Definition at line 178 of file [mgparm.h](#).

8.6.2.28 proc_rank

```
int proc_rank
```

Rank of this processor

Definition at line 180 of file [mgparm.h](#).

8.6.2.29 proc_size

```
int proc_size
```

Total number of processors

Definition at line 182 of file [mgparm.h](#).

8.6.2.30 setasynch

```
int setasynch
```

Flag,

See also

[asynch](#)

Definition at line 187 of file [mgparm.h](#).

8.6.2.31 setcgcent

```
int setcgcent
```

Flag,

See also

[ccmeth](#)

Definition at line 161 of file [mgparm.h](#).

8.6.2.32 setcglen

```
int setcglen
```

Flag,

See also

[cglen](#)

Definition at line 153 of file [mgparm.h](#).

8.6.2.33 setchgm

```
int setchgm
```

Flag,

See also

[chgm](#)

Definition at line 123 of file [mgparm.h](#).

8.6.2.34 setdime

```
int setdime
```

Flag,

See also

[dime](#)

Definition at line 121 of file [mgparm.h](#).

8.6.2.35 setetol

```
int setetol
```

Flag,

See also

[etol](#)

Definition at line 132 of file [mgparm.h](#).

8.6.2.36 setfgcent

```
int setfgcent
```

Flag,

See also

[fcmeth](#)

Definition at line 167 of file [mgparm.h](#).

8.6.2.37 setfglen

```
int setfglen
```

Flag,

See also

[fglen](#)

Definition at line 155 of file [mgparm.h](#).

8.6.2.38 setgcent

```
int setgcent
```

Flag,

See also

[cmeth](#)

Definition at line 149 of file [mgparm.h](#).

8.6.2.39 setglen

```
int setglen
```

Flag,

See also

[glen](#)

Definition at line 136 of file [mgparm.h](#).

8.6.2.40 setgrid

```
int setgrid  
Flag,
```

See also

[grid](#)

Definition at line 134 of file [mgparm.h](#).

8.6.2.41 setmethod

```
int setmethod  
Flag,
```

See also

[method](#)

Definition at line 193 of file [mgparm.h](#).

8.6.2.42 setnlev

```
int setnlev  
Flag,
```

See also

[nlev](#)

Definition at line 130 of file [mgparm.h](#).

8.6.2.43 setnonlotype

```
int setnonlotype  
Flag,
```

See also

[nonlotype](#)

Definition at line 190 of file [mgparm.h](#).

8.6.2.44 setofrac

```
int setofrac  
Flag,
```

See also

[ofrac](#)

Definition at line 185 of file [mgparm.h](#).

8.6.2.45 setpdime

```
int setpdime  
Flag,
```

See also

[pdime](#)

Definition at line 179 of file [mgparm.h](#).

8.6.2.46 setrank

```
int setrank
Flag,
```

See also

[proc_rank](#)

Definition at line 181 of file [mgparm.h](#).

8.6.2.47 setsize

```
int setsize
Flag,
```

See also

[proc_size](#)

Definition at line 183 of file [mgparm.h](#).

8.6.2.48 setUseAqua

```
int setUseAqua
Flag,
```

See also

[useAqua](#)

Definition at line 196 of file [mgparm.h](#).

8.6.2.49 type

[MGparm_CalcType](#) type

What type of MG calculation?

Definition at line 116 of file [mgparm.h](#).

8.6.2.50 useAqua

```
int useAqua
```

Enable use of lpbe/aqua

Definition at line 195 of file [mgparm.h](#).

The documentation for this struct was generated from the following file:

- [src/generic/mgparm.h](#)

8.7 sNosh Struct Reference

Class for parsing fixed format input files.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/generic/nosh.h>
```

Data Fields

- [Nosh_calc](#) * [calc](#) [[NOSH_MAXCALC](#)]
- int [ncalc](#)
- [Nosh_calc](#) * [elec](#) [[NOSH_MAXCALC](#)]

- int [nelec](#)
- [NOSH_calc](#) * [apol](#) [[NOSH_MAXCALC](#)]
- int [napol](#)
- int [ispara](#)
- int [proc_rank](#)
- int [proc_size](#)
- int [bogus](#)
- int [elec2calc](#) [[NOSH_MAXCALC](#)]
- int [apol2calc](#) [[NOSH_MAXCALC](#)]
- int [nmol](#)
- char [molpath](#) [[NOSH_MAXMOL](#)][[VMAX_ARGLEN](#)]
- [NOSH_MolFormat](#) [molfmt](#) [[NOSH_MAXMOL](#)]
- [Valist](#) * [alist](#) [[NOSH_MAXMOL](#)]
- int [gotparm](#)
- char [parmpath](#) [[VMAX_ARGLEN](#)]
- [NOSH_ParmFormat](#) [parmfmt](#)
- int [ndiel](#)
- char [dielXpath](#) [[NOSH_MAXMOL](#)][[VMAX_ARGLEN](#)]
- char [dielYpath](#) [[NOSH_MAXMOL](#)][[VMAX_ARGLEN](#)]
- char [dielZpath](#) [[NOSH_MAXMOL](#)][[VMAX_ARGLEN](#)]
- [Vdata_Format](#) [dielfmt](#) [[NOSH_MAXMOL](#)]
- int [nkappa](#)
- char [kappapath](#) [[NOSH_MAXMOL](#)][[VMAX_ARGLEN](#)]
- [Vdata_Format](#) [kappafmt](#) [[NOSH_MAXMOL](#)]
- int [npot](#)
- char [potpath](#) [[NOSH_MAXMOL](#)][[VMAX_ARGLEN](#)]
- [Vdata_Format](#) [potfmt](#) [[NOSH_MAXMOL](#)]
- int [ncharge](#)
- char [chargepath](#) [[NOSH_MAXMOL](#)][[VMAX_ARGLEN](#)]
- [Vdata_Format](#) [chargefmt](#) [[NOSH_MAXMOL](#)]
- int [nmesh](#)
- char [meshpath](#) [[NOSH_MAXMOL](#)][[VMAX_ARGLEN](#)]
- [Vdata_Format](#) [meshfmt](#) [[NOSH_MAXMOL](#)]
- int [nprint](#)
- [NOSH_PrintType](#) [printwhat](#) [[NOSH_MAXPRINT](#)]
- int [printnarg](#) [[NOSH_MAXPRINT](#)]
- int [printcalc](#) [[NOSH_MAXPRINT](#)][[NOSH_MAXPOP](#)]
- int [printop](#) [[NOSH_MAXPRINT](#)][[NOSH_MAXPOP](#)]
- int [parsed](#)
- char [elecname](#) [[NOSH_MAXCALC](#)][[VMAX_ARGLEN](#)]
- char [apolname](#) [[NOSH_MAXCALC](#)][[VMAX_ARGLEN](#)]

8.7.1 Detailed Description

Class for parsing fixed format input files.

Author

Nathan Baker

Definition at line 195 of file [nosh.h](#).

8.7.2 Field Documentation

8.7.2.1 alist

`Valist* alist[NOSH_MAXMOL]`

Molecules for calculation (can be used in setting mesh centers)

Definition at line 234 of file [nosh.h](#).

8.7.2.2 apol

`NOSH_calc* apol[NOSH_MAXCALC]`

The array of calculation objects corresponding to APOLAR statements read in the input file. Compare to [sNOsh::calc](#)

Definition at line 208 of file [nosh.h](#).

8.7.2.3 apol2calc

`int apol2calc[NOSH_MAXCALC]`

(see `elec2calc`)

Definition at line 229 of file [nosh.h](#).

8.7.2.4 apolname

`char apolname[NOSH_MAXCALC][VMAX_ARGLEN]`

Optional user-specified name for APOLAR statement

Definition at line 269 of file [nosh.h](#).

8.7.2.5 bogus

`int bogus`

A flag which tells routines using NOsh that this particular NOsh is broken – useful for parallel focusing calculations where the user gave us too many processors (1 => ignore this NOsh; 0 => this NOsh is OK)

Definition at line 217 of file [nosh.h](#).

8.7.2.6 calc

`NOSH_calc* calc[NOSH_MAXCALC]`

The array of calculation objects corresponding to actual calculations performed by the code. Compare to [sNOsh::elec](#)

Definition at line 197 of file [nosh.h](#).

8.7.2.7 chargefmt

`Vdata_Format chargefmt[NOSH_MAXMOL]`

Charge maps fileformats

Definition at line 255 of file [nosh.h](#).

8.7.2.8 chargepath

`char chargepath[NOSH_MAXMOL][VMAX_ARGLEN]`

Paths to charge map files

Definition at line 254 of file [nosh.h](#).

8.7.2.9 dielfmt

`Vdata_Format dielfmt[NOSH_MAXMOL]`

Dielectric maps file formats

Definition at line 246 of file [nosh.h](#).

8.7.2.10 dielXpath

```
char dielXpath[NOSH_MAXMOL][VMAX_ARGLEN]
```

Paths to x-shifted dielectric map files

Definition at line 240 of file [nosh.h](#).

8.7.2.11 dielYpath

```
char dielYpath[NOSH_MAXMOL][VMAX_ARGLEN]
```

Paths to y-shifted dielectric map files

Definition at line 242 of file [nosh.h](#).

8.7.2.12 dielZpath

```
char dielZpath[NOSH_MAXMOL][VMAX_ARGLEN]
```

Paths to z-shifted dielectric map files

Definition at line 244 of file [nosh.h](#).

8.7.2.13 elec

```
NOSH_calc* elec[NOSH_MAXCALC]
```

The array of calculation objects corresponding to ELEC statements read in the input file. Compare to [sNOsh::calc](#)

Definition at line 202 of file [nosh.h](#).

8.7.2.14 elec2calc

```
int elec2calc[NOSH_MAXCALC]
```

A mapping between ELEC statements which appear in the input file and calc objects stored above. Since we allow both normal and focused multigrid, there isn't a 1-to-1 correspondence between ELEC statements and actual calculations. This can really confuse operations which work on specific calculations further down the road (like PRINT). Therefore this array is the initial point of entry for any calculation-specific operation. It points to a specific entry in the calc array.

Definition at line 221 of file [nosh.h](#).

8.7.2.15 elecname

```
char elecname[NOSH_MAXCALC][VMAX_ARGLEN]
```

Optional user-specified name for ELEC statement

Definition at line 267 of file [nosh.h](#).

8.7.2.16 gotparm

```
int gotparm
```

Either have (1) or don't have (0) parm

Definition at line 236 of file [nosh.h](#).

8.7.2.17 ispara

```
int ispara
```

1 => is a parallel calculation, 0 => is not

Definition at line 214 of file [nosh.h](#).

8.7.2.18 kappafmt

```
Vdata_Format kappafmt[NOSH_MAXMOL]
```

Kappa maps file formats

Definition at line 249 of file [nosh.h](#).

8.7.2.19 kappapath

```
char kappapath[NOSH_MAXMOL] [VMAX_ARGLEN]
```

Paths to kappa map files

Definition at line 248 of file [nosh.h](#).

8.7.2.20 meshfmt

```
Vdata_Format meshfmt[NOSH_MAXMOL]
```

Mesh fileformats

Definition at line 258 of file [nosh.h](#).

8.7.2.21 meshpath

```
char meshpath[NOSH_MAXMOL] [VMAX_ARGLEN]
```

Paths to mesh files

Definition at line 257 of file [nosh.h](#).

8.7.2.22 molfmt

```
Nosh_MolFormat molfmt[NOSH_MAXMOL]
```

Mol files formats

Definition at line 233 of file [nosh.h](#).

8.7.2.23 molpath

```
char molpath[NOSH_MAXMOL] [VMAX_ARGLEN]
```

Paths to mol files

Definition at line 232 of file [nosh.h](#).

8.7.2.24 napol

```
int napol
```

The number of apolar statements in the input file and in the apolar array

Definition at line 211 of file [nosh.h](#).

8.7.2.25 ncalc

```
int ncalc
```

The number of calculations in the calc array

Definition at line 200 of file [nosh.h](#).

8.7.2.26 ncharge

```
int ncharge
```

Number of charge maps

Definition at line 253 of file [nosh.h](#).

8.7.2.27 ndiel

```
int ndiel
```

Number of dielectric maps

Definition at line 239 of file [nosh.h](#).

8.7.2.28 nelec

```
int nelec
```

The number of elec statements in the input file and in the elec array

Definition at line 205 of file [nosh.h](#).

8.7.2.29 nkappa

```
int nkappa
```

Number of kappa maps

Definition at line 247 of file [nosh.h](#).

8.7.2.30 nmesh

```
int nmesh
```

Number of meshes

Definition at line 256 of file [nosh.h](#).

8.7.2.31 nmol

```
int nmol
```

Number of molecules

Definition at line 231 of file [nosh.h](#).

8.7.2.32 npot

```
int npot
```

Number of potential maps

Definition at line 250 of file [nosh.h](#).

8.7.2.33 nprint

```
int nprint
```

How many print sections?

Definition at line 259 of file [nosh.h](#).

8.7.2.34 parmfmt

```
NOsh_ParmFormat parmfmt
```

Parm file format

Definition at line 238 of file [nosh.h](#).

8.7.2.35 parmpath

```
char parmpath[VMAX_ARGLLEN]
```

Paths to parm file

Definition at line 237 of file [nosh.h](#).

8.7.2.36 parsed

```
int parsed
```

Have we parsed an input file yet?

Definition at line 266 of file [nosh.h](#).

8.7.2.37 potfmt

Vdata_Format potfmt[NOSH_MAXMOL]

Potential maps file formats

Definition at line 252 of file [nosh.h](#).

8.7.2.38 potpath

char potpath[NOSH_MAXMOL][VMAX_ARGLEN]

Paths to potential map files

Definition at line 251 of file [nosh.h](#).

8.7.2.39 printcalc

int printcalc[NOSH_MAXPRINT][NOSH_MAXPOP]

ELEC id (see elec2calc)

Definition at line 263 of file [nosh.h](#).

8.7.2.40 printnarg

int printnarg[NOSH_MAXPRINT]

How many arguments in energy list

Definition at line 262 of file [nosh.h](#).

8.7.2.41 printop

int printop[NOSH_MAXPRINT][NOSH_MAXPOP]

Operation id (0 = add, 1 = subtract)

Definition at line 264 of file [nosh.h](#).

8.7.2.42 printwhat

Nosh_PrintType printwhat[NOSH_MAXPRINT]

What do we print:

- 0 = energy,
- 1 = force

Definition at line 260 of file [nosh.h](#).

8.7.2.43 proc_rank

int proc_rank

Processor rank in parallel calculation

Definition at line 215 of file [nosh.h](#).

8.7.2.44 proc_size

int proc_size

Number of processors in parallel calculation

Definition at line 216 of file [nosh.h](#).

The documentation for this struct was generated from the following file:

- [src/generic/nosh.h](#)

8.8 sNosh_calc Struct Reference

Calculation class for use when parsing fixed format input files.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/generic/nosh.h>
```

Data Fields

- [MGparm](#) * [mgparm](#)
- [FEMparm](#) * [femparm](#)
- [BEMparm](#) * [bemparm](#)
- [GEOFLOWparm](#) * [geoflowparm](#)
- [PBAMparm](#) * [pbamparm](#)
- [PBSAMparm](#) * [pbsamparm](#)
- [PBEparm](#) * [pbeparm](#)
- [APOLparm](#) * [apolparm](#)
- [NOsh_CalcType](#) [calctype](#)

8.8.1 Detailed Description

Calculation class for use when parsing fixed format input files.

Author

Nathan Baker

Definition at line 172 of file [nosh.h](#).

8.8.2 Field Documentation

8.8.2.1 apolparm

[APOLparm](#)* [apolparm](#)

Non-polar parameters

Definition at line 180 of file [nosh.h](#).

8.8.2.2 bemparm

[BEMparm](#)* [bemparm](#)

boundary element (tabi) parameters

Definition at line 175 of file [nosh.h](#).

8.8.2.3 calctype

[NOsh_CalcType](#) [calctype](#)

Calculation type

Definition at line 181 of file [nosh.h](#).

8.8.2.4 femparm

[FEMparm](#)* [femparm](#)

Finite element parameters

Definition at line 174 of file [nosh.h](#).

8.8.2.5 geoflowparm

`GEOFLOWparm*` geoflowparm

Geometric Flow Solver

Definition at line 176 of file [nosh.h](#).

8.8.2.6 mgparm

`MGparm*` mgparm

Multigrid parameters

Definition at line 173 of file [nosh.h](#).

8.8.2.7 pbamparm

`PBAMparm*` pbamparm

Analytical Poisson-Boltzmann Solver

Definition at line 177 of file [nosh.h](#).

8.8.2.8 pbeparm

`PBEparm*` pbeparm

Generic PBE parameters

Definition at line 179 of file [nosh.h](#).

8.8.2.9 pbsamparm

`PBSAMparm*` pbsamparm

Semi-Analytical Poisson-Boltzmann Solver

Definition at line 178 of file [nosh.h](#).

The documentation for this struct was generated from the following file:

- [src/generic/nosh.h](#)

8.9 sPBAMparm Struct Reference

Parameter structure for PBAM-specific variables from input files.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/generic/pbamparm.h>
```

Data Fields

- `PBAMparm_CalcType` type
- int `parsed`
- double `salt`
- int `setsalt`
- char `runtype` [CHR_MAXLEN]
- int `setruntype`
- char `runname` [CHR_MAXLEN]
- int `setrunname`
- int `setrandorient`
- double `pbcboxlen`
- int `setpbcs`
- char `units` [CHR_MAXLEN]
- int `setunits`
- int `gridpt`

- int [setgridpt](#)
- char [map3dname](#) [CHR_MAXLEN]
- int [set3dmap](#)
- char [grid2Dname](#) [PBAMPARM_MAXWRITE][CHR_MAXLEN]
- char [grid2Dax](#) [PBAMPARM_MAXWRITE][CHR_MAXLEN]
- double [grid2Dloc](#) [PBAMPARM_MAXWRITE]
- int [grid2Dct](#)
- int [setgrid2Dname](#)
- char [dxname](#) [CHR_MAXLEN]
- int [setdxname](#)
- int [ntraj](#)
- int [setntraj](#)
- char [termcombine](#) [CHR_MAXLEN]
- int [settermcombine](#)
- int [diffct](#)
- char [moveType](#) [PBAMPARM_MAXMOL][CHR_MAXLEN]
- double [transDiff](#) [PBAMPARM_MAXMOL]
- double [rotDiff](#) [PBAMPARM_MAXMOL]
- int [termct](#)
- int [setterm](#)
- char [termnam](#) [PBAMPARM_MAXWRITE][CHR_MAXLEN]
- int [termnu](#) [PBAMPARM_MAXWRITE][1]
- double [termVal](#) [PBAMPARM_MAXWRITE]
- char [confil](#) [PBAMPARM_MAXWRITE][CHR_MAXLEN]
- double [conpad](#) [PBAMPARM_MAXWRITE]
- int [confilct](#)
- int [setxyz](#)
- int [xyzct](#) [PBAMPARM_MAXMOL]
- char [xyzfil](#) [PBAMPARM_MAXMOL][PBAMPARM_MAXWRITE][CHR_MAXLEN]

8.9.1 Detailed Description

Parameter structure for PBAM-specific variables from input files.

Author

Andrew Stevens, Kyle Monson

Note

If you add/delete/change something in this class, the member functions – especially `PBAMParm_copy` – must be modified accordingly

Definition at line 105 of file [pbamparm.h](#).

8.9.2 Field Documentation

8.9.2.1 `confil`

`char confil [PBAMPARM_MAXWRITE] [CHR_MAXLEN]`

Definition at line 175 of file [pbamparm.h](#).

8.9.2.2 confilct

```
int confilct
```

Definition at line 177 of file [pbamparm.h](#).

8.9.2.3 conpad

```
double conpad[PBAMPARM_MAXWRITE]
```

Definition at line 176 of file [pbamparm.h](#).

8.9.2.4 diffct

```
int diffct
```

Definition at line 164 of file [pbamparm.h](#).

8.9.2.5 dxname

```
char dxname[CHR_MAXLEN]
```

Definition at line 152 of file [pbamparm.h](#).

8.9.2.6 grid2Dax

```
char grid2Dax[PBAMPARM_MAXWRITE][CHR_MAXLEN]
```

Definition at line 146 of file [pbamparm.h](#).

8.9.2.7 grid2Dct

```
int grid2Dct
```

Definition at line 148 of file [pbamparm.h](#).

8.9.2.8 grid2Dloc

```
double grid2Dloc[PBAMPARM_MAXWRITE]
```

Definition at line 147 of file [pbamparm.h](#).

8.9.2.9 grid2Dname

```
char grid2Dname[PBAMPARM_MAXWRITE][CHR_MAXLEN]
```

Definition at line 145 of file [pbamparm.h](#).

8.9.2.10 gridpt

```
int gridpt
```

Definition at line 137 of file [pbamparm.h](#).

8.9.2.11 map3dname

```
char map3dname[CHR_MAXLEN]
```

Definition at line 141 of file [pbamparm.h](#).

8.9.2.12 moveType

```
char moveType[PBAMPARM_MAXMOL][CHR_MAXLEN]
```

Definition at line 165 of file [pbamparm.h](#).

8.9.2.13 ntraj

```
int ntraj
```

Definition at line 158 of file [pbamparm.h](#).

8.9.2.14 parsed

```
int parsed
```

Has this structure been filled? (0 = no, 1 = yes)

Definition at line 108 of file [pbamparm.h](#).

8.9.2.15 pbcboxlen

```
double pbcboxlen
```

Definition at line 126 of file [pbamparm.h](#).

8.9.2.16 rotDiff

```
double rotDiff[PBAMPARM_MAXMOL]
```

Definition at line 167 of file [pbamparm.h](#).

8.9.2.17 runname

```
char runname[CHR_MAXLEN]
```

Definition at line 119 of file [pbamparm.h](#).

8.9.2.18 runtype

```
char runtype[CHR_MAXLEN]
```

Definition at line 115 of file [pbamparm.h](#).

8.9.2.19 salt

```
double salt
```

Definition at line 111 of file [pbamparm.h](#).

8.9.2.20 set3dmap

```
int set3dmap
```

Definition at line 142 of file [pbamparm.h](#).

8.9.2.21 setdxname

```
int setdxname
```

Definition at line 153 of file [pbamparm.h](#).

8.9.2.22 setgrid2Dname

```
int setgrid2Dname
```

Definition at line 149 of file [pbamparm.h](#).

8.9.2.23 setgridpt

```
int setgridpt
```

Definition at line 138 of file [pbamparm.h](#).

8.9.2.24 setntraj

```
int setntraj
```

Definition at line 159 of file [pbamparm.h](#).

8.9.2.25 setpbcs

```
int setpbcs
```

Definition at line 127 of file [pbamparm.h](#).

8.9.2.26 setrandorient

```
int setrandorient
```

Definition at line 123 of file [pbamparm.h](#).

8.9.2.27 setrunname

```
int setrunname
```

Definition at line 120 of file [pbamparm.h](#).

8.9.2.28 setruntype

```
int setruntype
```

Definition at line 116 of file [pbamparm.h](#).

8.9.2.29 setsalt

```
int setsalt
```

Definition at line 112 of file [pbamparm.h](#).

8.9.2.30 setterm

```
int setterm
```

Definition at line 170 of file [pbamparm.h](#).

8.9.2.31 settermcombine

```
int settermcombine
```

Definition at line 162 of file [pbamparm.h](#).

8.9.2.32 setunits

```
int setunits
```

Definition at line 131 of file [pbamparm.h](#).

8.9.2.33 setxyz

```
int setxyz
```

Definition at line 179 of file [pbamparm.h](#).

8.9.2.34 termcombine

```
char termcombine[CHR_MAXLEN]
```

Definition at line 161 of file [pbamparm.h](#).

8.9.2.35 termct

```
int termct
```

Definition at line 169 of file [pbamparm.h](#).

8.9.2.36 termnam

```
char termnam[PBAMPARM_MAXWRITE][CHR_MAXLEN]
```

Definition at line 172 of file [pbamparm.h](#).

8.9.2.37 termnu

```
int termnu[PBAMPARM_MAXWRITE][1]
```

Definition at line 173 of file [pbamparm.h](#).

8.9.2.38 termVal

```
double termVal[PBAMPARM_MAXWRITE]
```

Definition at line 174 of file [pbamparm.h](#).

8.9.2.39 transDiff

```
double transDiff[PBAMPARM_MAXMOL]
```

Definition at line 166 of file [pbamparm.h](#).

8.9.2.40 type

[PBAMparm_CalcType](#) type

What type of PBAM calculation?

Definition at line 107 of file [pbamparm.h](#).

8.9.2.41 units

```
char units[CHR_MAXLEN]
```

Definition at line 130 of file [pbamparm.h](#).

8.9.2.42 xyzct

```
int xyzct[PBAMPARM_MAXMOL]
```

Definition at line 180 of file [pbamparm.h](#).

8.9.2.43 xyzfil

```
char xyzfil[PBAMPARM_MAXMOL][PBAMPARM_MAXWRITE][CHR_MAXLEN]
```

Definition at line 181 of file [pbamparm.h](#).

The documentation for this struct was generated from the following file:

- [src/generic/pbamparm.h](#)

8.10 sPBEparm Struct Reference

Parameter structure for PBE variables from input files.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/generic/pbeparm.h>
```

Data Fields

- int [molid](#)
- int [setmolid](#)
- int [useDielMap](#)
- int [dielMapID](#)
- int [useKappaMap](#)
- int [kappaMapID](#)
- int [usePotMap](#)
- int [potMapID](#)
- int [useChargeMap](#)
- int [chargeMapID](#)
- [Vhal_PBEType](#) [pbetype](#)
- int [setpbetype](#)
- [Vbcfl](#) [bcfl](#)
- int [setbcfl](#)
- int [nion](#)
- int [setnion](#)
- double [ionq](#) [MAXION]
- double [ionc](#) [MAXION]
- double [ionr](#) [MAXION]
- int [setion](#) [MAXION]
- double [pdie](#)
- int [setpdie](#)
- double [sdens](#)
- int [setsdens](#)
- double [sdie](#)
- int [setsdie](#)
- [Vsurf_Meth](#) [srfm](#)
- int [setsrfm](#)
- double [srad](#)
- int [setsrad](#)
- double [swin](#)
- int [setswin](#)
- double [temp](#)
- int [settemp](#)
- double [smsize](#)
- int [setsmsize](#)
- double [smvolume](#)
- int [setsmvolume](#)
- [PBEparm_calcEnergy](#) [calcenergy](#)
- int [setcalcenergy](#)
- [PBEparm_calcForce](#) [calcforce](#)
- int [setcalcforce](#)
- double [zmem](#)
- int [setzmem](#)
- double [Lmem](#)
- int [setLmem](#)
- double [mdie](#)
- int [setmdie](#)
- double [memv](#)

- int [setmemv](#)
- int [numwrite](#)
- char [writestem](#) [PBEPARM_MAXWRITE][VMAX_ARGLEN]
- Vdata_Type [writetype](#) [PBEPARM_MAXWRITE]
- Vdata_Format [writefmt](#) [PBEPARM_MAXWRITE]
- int [writemat](#)
- int [setwritemat](#)
- char [writematstem](#) [VMAX_ARGLEN]
- int [writematflag](#)
- char [pbam_3dmapstem](#) [VMAX_ARGLEN]
- int [pbam_3dmapflag](#)
- int [parsed](#)

8.10.1 Detailed Description

Parameter structure for PBE variables from input files.

Author

Nathan Baker

Note

If you add/delete/change something in this class, the member functions – especially `PBEparm_copy` – must be modified accordingly

Definition at line 117 of file [pbeparm.h](#).

8.10.2 Field Documentation

8.10.2.1 `bconf`

[Vbconf](#) `bconf`

Boundary condition method

Definition at line 136 of file [pbeparm.h](#).

8.10.2.2 `calcenergy`

[PBEparm_calcEnergy](#) `calcenergy`

Energy calculation flag

Definition at line 165 of file [pbeparm.h](#).

8.10.2.3 `calcforce`

[PBEparm_calcForce](#) `calcforce`

Atomic forces calculation

Definition at line 167 of file [pbeparm.h](#).

8.10.2.4 `chargeMapID`

`int chargeMapID`

Charge distribution map ID (if used)

Definition at line 133 of file [pbeparm.h](#).

8.10.2.5 dielMapID

```
int dielMapID
```

Dielectric map ID (if used)

Definition at line 123 of file [pbeparm.h](#).

8.10.2.6 ionc

```
double ionc[MAXION]
```

Counterion concentrations (in M)

Definition at line 141 of file [pbeparm.h](#).

8.10.2.7 ionq

```
double ionq[MAXION]
```

Counterion charges (in e)

Definition at line 140 of file [pbeparm.h](#).

8.10.2.8 ionr

```
double ionr[MAXION]
```

Counterion radii (in Å)

Definition at line 142 of file [pbeparm.h](#).

8.10.2.9 kappaMapID

```
int kappaMapID
```

Kappa map ID (if used)

Definition at line 126 of file [pbeparm.h](#).

8.10.2.10 Lmem

```
double Lmem
```

membrane width

Definition at line 176 of file [pbeparm.h](#).

8.10.2.11 mdie

```
double mdie
```

membrane dielectric constant

Definition at line 178 of file [pbeparm.h](#).

8.10.2.12 memv

```
double memv
```

Membrane potential

Definition at line 180 of file [pbeparm.h](#).

8.10.2.13 molid

```
int molid
```

Molecule ID to perform calculation on

Definition at line 119 of file [pbeparm.h](#).

8.10.2.14 nion

```
int nion
```

Number of counterion species

Definition at line 138 of file [pbeparm.h](#).

8.10.2.15 numwrite

```
int numwrite
```

Number of write statements encountered

Definition at line 185 of file [pbeparm.h](#).

8.10.2.16 parsed

```
int parsed
```

Has this been filled with anything other than the default values?

Definition at line 205 of file [pbeparm.h](#).

8.10.2.17 pbam_3dmapflag

```
int pbam_3dmapflag
```

Definition at line 203 of file [pbeparm.h](#).

8.10.2.18 pbam_3dmapstem

```
char pbam_3dmapstem[VMAX_ARGLEN]
```

Definition at line 202 of file [pbeparm.h](#).

8.10.2.19 pbetype

```
Vhal_PBEType pbetype
```

Which version of the PBE are we solving?

Definition at line 134 of file [pbeparm.h](#).

8.10.2.20 pdie

```
double pdie
```

Solute dielectric

Definition at line 144 of file [pbeparm.h](#).

8.10.2.21 potMapID

```
int potMapID
```

Kappa map ID (if used)

Definition at line 129 of file [pbeparm.h](#).

8.10.2.22 sdens

```
double sdens
```

Vacc sphere density

Definition at line 146 of file [pbeparm.h](#).

8.10.2.23 sdie

double sdie

Solvent dielectric

Definition at line 148 of file [pbeparm.h](#).

8.10.2.24 setbcfl

int setbcfl

Flag,

See also

[bcfl](#)

Definition at line 137 of file [pbeparm.h](#).

8.10.2.25 setcalcenergy

int setcalcenergy

Flag,

See also

[calcenergy](#)

Definition at line 166 of file [pbeparm.h](#).

8.10.2.26 setcalcforce

int setcalcforce

Flag,

See also

[calcforce](#)

Definition at line 168 of file [pbeparm.h](#).

8.10.2.27 setion

int setion[[MAXION](#)]

Flag,

See also

[ionq](#)

Definition at line 143 of file [pbeparm.h](#).

8.10.2.28 setLmem

int setLmem

Flag

Definition at line 177 of file [pbeparm.h](#).

8.10.2.29 setmdie

int setmdie

Flag

Definition at line 179 of file [pbeparm.h](#).

8.10.2.30 setmemv

```
int setmemv
```

Flag

Definition at line 181 of file [pbeparm.h](#).

8.10.2.31 setmolid

```
int setmolid
```

Flag,

See also

[molid](#)

Definition at line 120 of file [pbeparm.h](#).

8.10.2.32 setnion

```
int setnion
```

Flag,

See also

[nion](#)

Definition at line 139 of file [pbeparm.h](#).

8.10.2.33 setpbetype

```
int setpbetype
```

Flag,

See also

[pbetype](#)

Definition at line 135 of file [pbeparm.h](#).

8.10.2.34 setpdie

```
int setpdie
```

Flag,

See also

[pdie](#)

Definition at line 145 of file [pbeparm.h](#).

8.10.2.35 setsdens

```
int setsdens
```

Flag,

See also

[sdens](#)

Definition at line 147 of file [pbeparm.h](#).

8.10.2.36 setsdie

```
int setsdie
```

Flag,

See also

[sdie](#)

Definition at line 149 of file [pbeparm.h](#).

8.10.2.37 setsmsize

```
int setsmsize
```

Flag,

See also

[temp](#)

Definition at line 160 of file [pbeparm.h](#).

8.10.2.38 setsmvolume

```
int setsmvolume
```

Flag,

See also

[temp](#)

Definition at line 163 of file [pbeparm.h](#).

8.10.2.39 setsrad

```
int setsrad
```

Flag,

See also

[srad](#)

Definition at line 153 of file [pbeparm.h](#).

8.10.2.40 setsrfm

```
int setsrfm
```

Flag,

See also

[srfm](#)

Definition at line 151 of file [pbeparm.h](#).

8.10.2.41 setswin

```
int setswin
```

Flag,

See also

[swin](#)

Definition at line 155 of file [pbeparm.h](#).

8.10.2.42 settemp

int settemp
Flag,

See also

[temp](#)

Definition at line 157 of file [pbeparm.h](#).

8.10.2.43 setwritemat

int setwritemat
Flag,

See also

[writemat](#)

Definition at line 194 of file [pbeparm.h](#).

8.10.2.44 setzmem

int setzmem
Flag

Definition at line 175 of file [pbeparm.h](#).

8.10.2.45 smsize

double smsize
SMPBE size

Definition at line 159 of file [pbeparm.h](#).

8.10.2.46 smvolume

double smvolume
SMPBE size

Definition at line 162 of file [pbeparm.h](#).

8.10.2.47 srad

double srad
Solvent radius

Definition at line 152 of file [pbeparm.h](#).

8.10.2.48 srfm

Vsurf_Meth srfm
Surface calculation method

Definition at line 150 of file [pbeparm.h](#).

8.10.2.49 swin

double swin
Cubic spline window

Definition at line 154 of file [pbeparm.h](#).

8.10.2.50 temp

double temp

Temperature (in K)

Definition at line 156 of file [pbeparm.h](#).

8.10.2.51 useChargeMap

int useChargeMap

Indicates whether we use an external charge distribution map

Definition at line 131 of file [pbeparm.h](#).

8.10.2.52 useDielMap

int useDielMap

Indicates whether we use external dielectric maps (note plural)

Definition at line 121 of file [pbeparm.h](#).

8.10.2.53 useKappaMap

int useKappaMap

Indicates whether we use an external kappa map

Definition at line 124 of file [pbeparm.h](#).

8.10.2.54 usePotMap

int usePotMap

Indicates whether we use an external kappa map

Definition at line 127 of file [pbeparm.h](#).

8.10.2.55 writefmt

Vdata_Format writefmt[PBEPARM_MAXWRITE]

File format to write data in

Definition at line 189 of file [pbeparm.h](#).

8.10.2.56 writemat

int writemat

Write out the operator matrix?

- 0 => no
- 1 => yes

Definition at line 191 of file [pbeparm.h](#).

8.10.2.57 writematflag

int writematflag

What matrix should we write:

- 0 => Poisson (differential operator)
- 1 => Poisson-Boltzmann operator linearized around solution (if applicable)

Definition at line 196 of file [pbeparm.h](#).

8.10.2.58 writematstem

```
char writematstem[VMAX_ARGLEN]
```

File stem to write mat

Definition at line 195 of file [pbeparm.h](#).

8.10.2.59 writestem

```
char writestem[PBEPPARM_MAXWRITE] [VMAX_ARGLEN]
```

File stem to write data to

Definition at line 186 of file [pbeparm.h](#).

8.10.2.60 writetype

```
Vdata_Type writetype[PBEPPARM_MAXWRITE]
```

What data to write

Definition at line 188 of file [pbeparm.h](#).

8.10.2.61 zmem

```
double zmem
```

z value of membrane bottom

Definition at line 174 of file [pbeparm.h](#).

The documentation for this struct was generated from the following file:

- [src/generic/pbeparm.h](#)

8.11 sPBSAMParm Struct Reference

Parameter structure for PBSAM-specific variables from input files.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/generic/pbsamparm.h>
```

Data Fields

- [PBSAMParm_CalcType](#) type
- int [parsed](#)
- int [settolsp](#)
- double [tolsp](#)
- int [setmsms](#)
- double [probe_radius](#)
- double [density](#)
- int [setsurf](#)
- int [surfct](#)
- char [surffil](#) [PBSAMPARM_MAXMOL][[CHR_MAXLEN](#)]
- int [setimat](#)
- int [imatct](#)
- char [imatfil](#) [PBSAMPARM_MAXMOL][[CHR_MAXLEN](#)]
- int [setexp](#)
- int [expct](#)
- char [expfil](#) [PBSAMPARM_MAXMOL][[CHR_MAXLEN](#)]

8.11.1 Detailed Description

Parameter structure for PBSAM-specific variables from input files.

Author

Lisa Felberg

Note

If you add/delete/change something in this class, the member functions – especially `PBSAMparm_copy` – must be modified accordingly

Definition at line 105 of file [pbsamparm.h](#).

8.11.2 Field Documentation

8.11.2.1 density

`double density`

Definition at line 117 of file [pbsamparm.h](#).

8.11.2.2 expct

`int expct`

Definition at line 128 of file [pbsamparm.h](#).

8.11.2.3 expfil

`char expfil[PBSAMPARM_MAXMOL][CHR_MAXLEN]`

Definition at line 129 of file [pbsamparm.h](#).

8.11.2.4 imatct

`int imatct`

Definition at line 124 of file [pbsamparm.h](#).

8.11.2.5 imatfil

`char imatfil[PBSAMPARM_MAXMOL][CHR_MAXLEN]`

Definition at line 125 of file [pbsamparm.h](#).

8.11.2.6 parsed

`int parsed`

Has this structure been filled? (0 = no, 1 = yes)

Definition at line 108 of file [pbsamparm.h](#).

8.11.2.7 probe_radius

`double probe_radius`

Definition at line 116 of file [pbsamparm.h](#).

8.11.2.8 setexp

`int setexp`

Definition at line 127 of file [pbsamparm.h](#).

8.11.2.9 setimat

int setimat

Definition at line 123 of file [pbsamparm.h](#).

8.11.2.10 setmsms

int setmsms

Definition at line 115 of file [pbsamparm.h](#).

8.11.2.11 setsurf

int setsurf

Definition at line 119 of file [pbsamparm.h](#).

8.11.2.12 settolsp

int settolsp

Definition at line 112 of file [pbsamparm.h](#).

8.11.2.13 surfct

int surfct

Definition at line 120 of file [pbsamparm.h](#).

8.11.2.14 surffil

char surffil[PBSAMPARM_MAXMOL][CHR_MAXLEN]

Definition at line 121 of file [pbsamparm.h](#).

8.11.2.15 tolspace

double tolspace

Definition at line 113 of file [pbsamparm.h](#).

8.11.2.16 type

[PBSAMParm_CalcType](#) type

What type of PBSAM calculation?

Definition at line 107 of file [pbsamparm.h](#).

The documentation for this struct was generated from the following file:

- [src/generic/pbsamparm.h](#)

8.12 sVacc Struct Reference

Oracle for solvent- and ion-accessibility around a biomolecule.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/generic/vacc.h>
```

Data Fields

- Vmem * [mem](#)
- Valist * [alist](#)
- Vclist * [clist](#)
- int * [atomFlags](#)

- [VaccSurf](#) * [refSphere](#)
- [VaccSurf](#) ** [surf](#)
- Vset [acc](#)
- double [surf_density](#)

8.12.1 Detailed Description

Oracle for solvent- and ion-accessibility around a biomolecule.

Author

Nathan Baker

Definition at line 108 of file [vacc.h](#).

8.12.2 Field Documentation

8.12.2.1 acc

Vset [acc](#)

An integer array (to be treated as bitfields) of Vset type with length equal to the number of vertices in the mesh

Definition at line 120 of file [vacc.h](#).

8.12.2.2 alist

[Valist](#)* [alist](#)

Valist structure for list of atoms

Definition at line 111 of file [vacc.h](#).

8.12.2.3 atomFlags

int* [atomFlags](#)

Array of boolean flags of length [Valist_getNumberAtoms\(thee->alist\)](#) to prevent double-counting atoms during calculations

Definition at line 113 of file [vacc.h](#).

8.12.2.4 clist

[Vclist](#)* [clist](#)

Vclist structure for atom cell list

Definition at line 112 of file [vacc.h](#).

8.12.2.5 mem

Vmem* [mem](#)

Memory management object for this class

Definition at line 110 of file [vacc.h](#).

8.12.2.6 refSphere

[VaccSurf](#)* [refSphere](#)

Reference sphere for SASA calculations

Definition at line 116 of file [vacc.h](#).

8.12.2.7 surf

`VaccSurf** surf`

Array of surface points for each atom; is not initialized until needed (test against VNULL to determine initialization state)
Definition at line 117 of file [vacc.h](#).

8.12.2.8 surf_density

`double surf_density`

Minimum solvent accessible surface point density (in pts/A²)

Definition at line 122 of file [vacc.h](#).

The documentation for this struct was generated from the following file:

- [src/generic/vacc.h](#)

8.13 sVaccSurf Struct Reference

Surface object list of per-atom surface points.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/generic/vacc.h>
```

Data Fields

- `Vmem * mem`
- `double * xpts`
- `double * ypts`
- `double * zpts`
- `char * bpts`
- `double area`
- `int npts`
- `double probe_radius`

8.13.1 Detailed Description

Surface object list of per-atom surface points.

Author

Nathan Baker

Definition at line 84 of file [vacc.h](#).

8.13.2 Field Documentation

8.13.2.1 area

`double area`

Area spanned by these points

Definition at line 91 of file [vacc.h](#).

8.13.2.2 bpts

`char* bpts`

Array of booleans indicating whether a point is (1) or is not (0) part of the surface

Definition at line 89 of file [vacc.h](#).

8.13.2.3 mem

Vmem* mem

Memory object

Definition at line 85 of file [vacc.h](#).

8.13.2.4 npts

int npts

Length of thee->xpts, ypts, zpts arrays

Definition at line 92 of file [vacc.h](#).

8.13.2.5 probe_radius

double probe_radius

Probe radius (A) with which this surface was constructed

Definition at line 93 of file [vacc.h](#).

8.13.2.6 xpts

double* xpts

Array of point x-locations

Definition at line 86 of file [vacc.h](#).

8.13.2.7 ypts

double* ypts

Array of point y-locations

Definition at line 87 of file [vacc.h](#).

8.13.2.8 zpts

double* zpts

Array of point z-locations

Definition at line 88 of file [vacc.h](#).

The documentation for this struct was generated from the following file:

- [src/generic/vacc.h](#)

8.14 sValist Struct Reference

Container class for list of atom objects.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/generic/valist.h>
```

Data Fields

- int [number](#)
- double [center](#) [3]
- double [mincrd](#) [3]
- double [maxcrd](#) [3]
- double [maxrad](#)
- double [charge](#)
- [Vatom](#) * [atoms](#)
- [Vmem](#) * [vmem](#)

8.14.1 Detailed Description

Container class for list of atom objects.

Author

Nathan Baker

Definition at line 78 of file [valist.h](#).

8.14.2 Field Documentation

8.14.2.1 atoms

`Vatom*` atoms

Atom list

Definition at line 86 of file [valist.h](#).

8.14.2.2 center

`double` center[3]

Molecule center (xmin - xmax)/2, etc.

Definition at line 81 of file [valist.h](#).

8.14.2.3 charge

`double` charge

Net charge

Definition at line 85 of file [valist.h](#).

8.14.2.4 maxcrd

`double` maxcrd[3]

Maximum coordinates

Definition at line 83 of file [valist.h](#).

8.14.2.5 maxrad

`double` maxrad

Maximum radius

Definition at line 84 of file [valist.h](#).

8.14.2.6 mincrd

`double` mincrd[3]

Minimum coordinates

Definition at line 82 of file [valist.h](#).

8.14.2.7 number

`int` number

Number of atoms in list

Definition at line 80 of file [valist.h](#).

8.14.2.8 vmem

Vmem* vmem

Memory management object

Definition at line 87 of file [valist.h](#).

The documentation for this struct was generated from the following file:

- [src/generic/valist.h](#)

8.15 sVatom Struct Reference

Contains public data members for Vatom class/module.

#include [</builddir/build/BUILD/apbs-3.0.0/src/generic/vatom.h>](#)

Data Fields

- double [position](#) [3]
- double [radius](#)
- double [charge](#)
- double [partID](#)
- double [epsilon](#)
- int [id](#)
- char [resName](#) [VMAX_RECLEN]
- char [atomName](#) [VMAX_RECLEN]

8.15.1 Detailed Description

Contains public data members for Vatom class/module.

Author

Nathan Baker, David Gohara, Mike Schneiders

Definition at line 84 of file [vatom.h](#).

8.15.2 Field Documentation

8.15.2.1 atomName

char [atomName](#) [VMAX_RECLEN]

Atom name from PDB/PDR file

Definition at line 98 of file [vatom.h](#).

8.15.2.2 charge

double [charge](#)

Atomic charge

Definition at line 88 of file [vatom.h](#).

8.15.2.3 epsilon

double [epsilon](#)

Epsilon value for WCA calculations

Definition at line 91 of file [vatom.h](#).

8.15.2.4 id

```
int id
```

Atomic ID; this should be a unique non-negative integer assigned based on the index of the atom in a Valist atom array
Definition at line 93 of file [vatom.h](#).

8.15.2.5 partID

```
double partID
```

Partition value for assigning atoms to particular processors and/or partitions

Definition at line 89 of file [vatom.h](#).

8.15.2.6 position

```
double position[3]
```

Atomic position

Definition at line 86 of file [vatom.h](#).

8.15.2.7 radius

```
double radius
```

Atomic radius

Definition at line 87 of file [vatom.h](#).

8.15.2.8 resName

```
char resName[VMAX_RECLEN]
```

Residue name from PDB/PQR file

Definition at line 97 of file [vatom.h](#).

The documentation for this struct was generated from the following file:

- [src/generic/vatom.h](#)

8.16 sVclist Struct Reference

Atom cell list.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/generic/vclist.h>
```

Data Fields

- Vmem * [vmem](#)
- Valist * [alist](#)
- Vclist_DomainMode [mode](#)
- int [npts](#) [[VAPBS_DIM](#)]
- int [n](#)
- double [max_radius](#)
- VclistCell * [cells](#)
- double [lower_corner](#) [[VAPBS_DIM](#)]
- double [upper_corner](#) [[VAPBS_DIM](#)]
- double [spacs](#) [[VAPBS_DIM](#)]

8.16.1 Detailed Description

Atom cell list.

Author

Nathan Baker

Definition at line 117 of file [vclist.h](#).

8.16.2 Field Documentation

8.16.2.1 alist

`Valist*` alist

Original Valist structure for list of atoms

Definition at line 120 of file [vclist.h](#).

8.16.2.2 cells

`VclistCell*` cells

Cell array of length thee->n

Definition at line 125 of file [vclist.h](#).

8.16.2.3 lower_corner

`double` lower_corner[VAPBS_DIM]

Hash table grid corner

Definition at line 126 of file [vclist.h](#).

8.16.2.4 max_radius

`double` max_radius

Maximum probe radius

Definition at line 124 of file [vclist.h](#).

8.16.2.5 mode

`Vclist_DomainMode` mode

How the cell list was constructed

Definition at line 121 of file [vclist.h](#).

8.16.2.6 n

`int` n

$n = n_x * n_z * n_y$

Definition at line 123 of file [vclist.h](#).

8.16.2.7 npts

`int` npts[VAPBS_DIM]

Hash table grid dimensions

Definition at line 122 of file [vclist.h](#).

8.16.2.8 spacs

```
double spacs[VAPBS_DIM]
```

Hash table grid spacings

Definition at line 128 of file [vclist.h](#).

8.16.2.9 upper_corner

```
double upper_corner[VAPBS_DIM]
```

Hash table grid corner

Definition at line 127 of file [vclist.h](#).

8.16.2.10 vmem

```
Vmem* vmem
```

Memory management object for this class

Definition at line 119 of file [vclist.h](#).

The documentation for this struct was generated from the following file:

- [src/generic/vclist.h](#)

8.17 sVclistCell Struct Reference

Atom cell list cell.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/generic/vclist.h>
```

Data Fields

- [Vatom](#) ** [atoms](#)
- int [natoms](#)

8.17.1 Detailed Description

Atom cell list cell.

Author

Nathan Baker

Definition at line 101 of file [vclist.h](#).

8.17.2 Field Documentation

8.17.2.1 atoms

```
Vatom** atoms
```

Array of atom objects associated with this cell

Definition at line 102 of file [vclist.h](#).

8.17.2.2 natoms

```
int natoms
```

Length of the->atoms array

Definition at line 103 of file [vclist.h](#).

The documentation for this struct was generated from the following file:

- [src/generic/vclist.h](#)

8.18 sVcsm Struct Reference

Charge-simplex map class.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/fem/vcsm.h>
```

Data Fields

- [Valist](#) * [alist](#)
- int [natom](#)
- Gem * [gm](#)
- int ** [sqm](#)
- int * [nsqm](#)
- int [nsimp](#)
- int [msimp](#)
- int ** [qsm](#)
- int * [nqsm](#)
- int [initFlag](#)
- Vmem * [vmem](#)

8.18.1 Detailed Description

Charge-simplex map class.

Author

Nathan Baker

Definition at line 89 of file [vcsm.h](#).

8.18.2 Field Documentation

8.18.2.1 alist

[Valist](#)* [alist](#)

Atom (charge) list

Definition at line 91 of file [vcsm.h](#).

8.18.2.2 gm

Gem* [gm](#)

Grid manager (container class for master vertex and simplex lists as well as prolongation operator for updating after refinement)

Definition at line 94 of file [vcsm.h](#).

8.18.2.3 initFlag

int [initFlag](#)

Indicates whether the maps have been initialized yet

Definition at line 112 of file [vcsm.h](#).

8.18.2.4 msimp

int [msimp](#)

The maximum number of entries that can be accomodated by [sqm](#) or [nsqm](#) – saves on realloc's

Definition at line 107 of file [vcsm.h](#).

8.18.2.5 natom

```
int natom
```

Size of thee->alist; redundant, but useful for convenience

Definition at line 92 of file [vcsn.h](#).

8.18.2.6 nqsm

```
int* nqsm
```

The length of the simplex lists in thee->qsm

Definition at line 111 of file [vcsn.h](#).

8.18.2.7 nsimp

```
int nsimp
```

The (currently used) length of sqm, nsqm – may not always be up-to-date with Gem

Definition at line 105 of file [vcsn.h](#).

8.18.2.8 nsqm

```
int* nsqm
```

The length of the charge lists in thee->sqm

Definition at line 104 of file [vcsn.h](#).

8.18.2.9 qsm

```
int** qsm
```

The inverse of sqm; the list of simplices associated with a given charge

Definition at line 109 of file [vcsn.h](#).

8.18.2.10 sqm

```
int** sqm
```

The map which gives the list charges associated with each simplex in gm->simplices. The indices of the first dimension are associated with the simplex ID's in Vgm. Each charge list (second dimension) contains entries corresponding to indices in thee->alist with lengths given in thee->nsqm

Definition at line 97 of file [vcsn.h](#).

8.18.2.11 vmem

```
Vmem* vmem
```

Memory management object

Definition at line 114 of file [vcsn.h](#).

The documentation for this struct was generated from the following file:

- [src/fem/vcsn.h](#)

8.19 sVfetk Struct Reference

Contains public data members for Vfetk class/module.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/fem/vfetk.h>
```

Data Fields

- Vmem * [vmem](#)
- Gem * [gm](#)
- AM * [am](#)
- Aprx * [aprx](#)
- PDE * [pde](#)
- Vpbe * [pbe](#)
- Vcsm * [csm](#)
- Vfetk_LsolvType lkey
- int [lmax](#)
- double [ltol](#)
- Vfetk_NsolvType nkey
- int [nmax](#)
- double [ntol](#)
- Vfetk_GuessType gues
- Vfetk_PrecType lprec
- int [pjac](#)
- PBEparm * [pbeparm](#)
- FEMparm * [feparm](#)
- Vhal_PBEType type
- int [level](#)

8.19.1 Detailed Description

Contains public data members for Vfetk class/module.

Author

Nathan Baker

Many of the routines and macros are borrowed from the [main.c](#) driver (written by Mike Holst) provided with the PMG code.

Definition at line [176](#) of file [vfetk.h](#).

8.19.2 Field Documentation

8.19.2.1 am

AM* [am](#)

Multilevel algebra manager.

Definition at line [182](#) of file [vfetk.h](#).

8.19.2.2 aprx

Aprx* [aprx](#)

Approximation manager.

Definition at line [183](#) of file [vfetk.h](#).

8.19.2.3 csm

Vcsm* [csm](#)

Charge-simplex map

Definition at line [186](#) of file [vfetk.h](#).

8.19.2.4 feparm

`FEMparm*` feparm

FEM-specific parameters

Definition at line 198 of file [vfetk.h](#).

8.19.2.5 gm

`Gem*` gm

Grid manager (container class for master vertex and simplex lists as well as prolongation operator for updating after refinement).

Definition at line 179 of file [vfetk.h](#).

8.19.2.6 gues

`Vfetk_GuessType` gues

Initial guess method

Definition at line 193 of file [vfetk.h](#).

8.19.2.7 level

`int` level

Refinement level (starts at 0)

Definition at line 200 of file [vfetk.h](#).

8.19.2.8 lkey

`Vfetk_LsolvType` lkey

Linear solver method

Definition at line 187 of file [vfetk.h](#).

8.19.2.9 lmax

`int` lmax

Maximum number of linear solver iterations

Definition at line 188 of file [vfetk.h](#).

8.19.2.10 lprec

`Vfetk_PrecType` lprec

Linear preconditioner

Definition at line 194 of file [vfetk.h](#).

8.19.2.11 ltol

`double` ltol

Residual tolerance for linear solver

Definition at line 189 of file [vfetk.h](#).

8.19.2.12 nkey

`Vfetk_NsolvType` nkey

Nonlinear solver method

Definition at line 190 of file [vfetk.h](#).

8.19.2.13 nmax

int nmax

Maximum number of nonlinear solver iterations

Definition at line 191 of file [vfetk.h](#).

8.19.2.14 ntol

double ntol

Residual tolerance for nonlinear solver

Definition at line 192 of file [vfetk.h](#).

8.19.2.15 pbe

Vpbe* pbe

Poisson-Boltzmann object

Definition at line 185 of file [vfetk.h](#).

8.19.2.16 pbeparm

PBEparm* pbeparm

Generic PB parameters

Definition at line 197 of file [vfetk.h](#).

8.19.2.17 pde

PDE* pde

FEtk PDE object

Definition at line 184 of file [vfetk.h](#).

8.19.2.18 pjac

int pjac

Flag to print the jacobians (usually set this to -1, please)

Definition at line 195 of file [vfetk.h](#).

8.19.2.19 type

Vhal_PBEType type

Version of PBE to solve

Definition at line 199 of file [vfetk.h](#).

8.19.2.20 vmem

Vmem* vmem

Memory management object

Definition at line 178 of file [vfetk.h](#).

The documentation for this struct was generated from the following file:

- [src/fem/vfetk.h](#)

8.20 sVfetk_LocalVar Struct Reference

Vfetk LocalVar subclass.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/fem/vfetk.h>
```

Data Fields

- double [nvec](#) [[VAPBS_DIM](#)]
- double [vx](#) [4][[VAPBS_DIM](#)]
- double [xq](#) [[VAPBS_DIM](#)]
- double [U](#) [[MAXV](#)]
- double [dU](#) [[MAXV](#)][[VAPBS_DIM](#)]
- double [W](#)
- double [dW](#) [[VAPBS_DIM](#)]
- double [d2W](#)
- int [sType](#)
- int [fType](#)
- double [A](#)
- double [F](#)
- double [B](#)
- double [DB](#)
- double [jumpDiel](#)
- [Vfetk](#) * [fetk](#)
- [Vgreen](#) * [green](#)
- int [initGreen](#)
- SS * [simp](#)
- VV * [verts](#) [4]
- int [nverts](#)
- double [ionConc](#) [[MAXION](#)]
- double [ionQ](#) [[MAXION](#)]
- double [ionRadii](#) [[MAXION](#)]
- double [zkappa2](#)
- double [zks2](#)
- double [ionstr](#)
- int [nion](#)
- double [Fu_v](#)
- double [DFu_wv](#)
- double [delta](#)
- double [u_D](#)
- double [u_T](#)

8.20.1 Detailed Description

Vfetk LocalVar subclass.

Author

Nathan Baker

Contains variables used when solving the PDE with FETk
Definition at line [215](#) of file [vfetk.h](#).

8.20.2 Field Documentation

8.20.2.1 A

double A

Second-order differential term

Definition at line [228](#) of file [vfetk.h](#).

8.20.2.2 B

double B

Entire ionic strength term

Definition at line 230 of file [vfetk.h](#).

8.20.2.3 d2W

double d2W

Coulomb regularization term Laplacian

Definition at line 223 of file [vfetk.h](#).

8.20.2.4 DB

double DB

Entire ionic strength term derivative

Definition at line 231 of file [vfetk.h](#).

8.20.2.5 delta

double delta

Store delta value

Definition at line 250 of file [vfetk.h](#).

8.20.2.6 DFu_wv

double DFu_wv

Store DFu_wv value

Definition at line 249 of file [vfetk.h](#).

8.20.2.7 dU

double dU[MAXV][VAPBS_DIM]

Solution gradient

Definition at line 220 of file [vfetk.h](#).

8.20.2.8 dW

double dW[VAPBS_DIM]

Coulomb regularization term gradient

Definition at line 222 of file [vfetk.h](#).

8.20.2.9 F

double F

RHS characteristic function value

Definition at line 229 of file [vfetk.h](#).

8.20.2.10 fetk

[Vfetk*](#) fetk

Pointer to the VFETK object

Definition at line 233 of file [vfetk.h](#).

8.20.2.11 fType

```
int fType
```

Face type

Definition at line 225 of file [vfetk.h](#).

8.20.2.12 Fu_v

```
double Fu_v
```

Store Fu_v value

Definition at line 248 of file [vfetk.h](#).

8.20.2.13 green

```
Vgreen* green
```

Pointer to a Green's function object

Definition at line 234 of file [vfetk.h](#).

8.20.2.14 initGreen

```
int initGreen
```

Boolean to designate whether Green's function has been initialized

Definition at line 235 of file [vfetk.h](#).

8.20.2.15 ionConc

```
double ionConc[MAXION]
```

Counterion species' concentrations

Definition at line 241 of file [vfetk.h](#).

8.20.2.16 ionQ

```
double ionQ[MAXION]
```

Counterion species' valencies

Definition at line 242 of file [vfetk.h](#).

8.20.2.17 ionRadii

```
double ionRadii[MAXION]
```

Counterion species' radii

Definition at line 243 of file [vfetk.h](#).

8.20.2.18 ionstr

```
double ionstr
```

Ionic strength parameters (M)

Definition at line 246 of file [vfetk.h](#).

8.20.2.19 jumpDiel

```
double jumpDiel
```

Dielectric value on one side of a simplex face

Definition at line 232 of file [vfetk.h](#).

8.20.2.20 nion

```
int nion
```

Number of ion species

Definition at line 247 of file [vfetk.h](#).

8.20.2.21 nvec

```
double nvec[VAPBS_DIM]
```

Normal vector for a simplex face

Definition at line 216 of file [vfetk.h](#).

8.20.2.22 nverts

```
int nverts
```

number of vertices in the simplex

Definition at line 240 of file [vfetk.h](#).

8.20.2.23 simp

```
SS* simp
```

Pointer to the latest simplex object; set in `initElement()` and `delta()`

Definition at line 237 of file [vfetk.h](#).

8.20.2.24 sType

```
int sType
```

Simplex type

Definition at line 224 of file [vfetk.h](#).

8.20.2.25 U

```
double U[MAXV]
```

Solution value

Definition at line 219 of file [vfetk.h](#).

8.20.2.26 u_D

```
double u_D
```

Store Dirichlet value

Definition at line 251 of file [vfetk.h](#).

8.20.2.27 u_T

```
double u_T
```

Store true value

Definition at line 252 of file [vfetk.h](#).

8.20.2.28 verts

```
VV* verts[4]
```

Pointer to the latest vertices; set in `initElement`

Definition at line 239 of file [vfetk.h](#).

8.20.2.29 vx

```
double vx[4][VAPBS_DIM]
```

Vertex coordinates

Definition at line 217 of file [vfetk.h](#).

8.20.2.30 W

```
double W
```

Coulomb regularization term scalar value

Definition at line 221 of file [vfetk.h](#).

8.20.2.31 xq

```
double xq[VAPBS_DIM]
```

Quadrature pt

Definition at line 218 of file [vfetk.h](#).

8.20.2.32 zkappa2

```
double zkappa2
```

Ionic strength parameters

Definition at line 244 of file [vfetk.h](#).

8.20.2.33 zks2

```
double zks2
```

Ionic strength parameters

Definition at line 245 of file [vfetk.h](#).

The documentation for this struct was generated from the following file:

- [src/fem/vfetk.h](#)

8.21 sVgreen Struct Reference

Contains public data members for Vgreen class/module.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/generic/vgreen.h>
```

Data Fields

- [Valist](#) * [alist](#)
- [Vmem](#) * [vmem](#)
- [double](#) * [xp](#)
- [double](#) * [yp](#)
- [double](#) * [zp](#)
- [double](#) * [qp](#)
- [int](#) [np](#)

8.21.1 Detailed Description

Contains public data members for Vgreen class/module.

Author

Nathan Baker

Definition at line 82 of file [vgreen.h](#).

8.21.2 Field Documentation

8.21.2.1 alist

`Valist* alist`

Atom (charge) list for Green's function

Definition at line 84 of file [vgreen.h](#).

8.21.2.2 np

`int np`

Set to size of above arrays

Definition at line 94 of file [vgreen.h](#).

8.21.2.3 qp

`double* qp`

Array of particle charges for use with treecode routines

Definition at line 92 of file [vgreen.h](#).

8.21.2.4 vmem

`Vmem* vmem`

Memory management object

Definition at line 85 of file [vgreen.h](#).

8.21.2.5 xp

`double* xp`

Array of particle x-coordinates for use with treecode routines

Definition at line 86 of file [vgreen.h](#).

8.21.2.6 yp

`double* yp`

Array of particle y-coordinates for use with treecode routines

Definition at line 88 of file [vgreen.h](#).

8.21.2.7 zp

`double* zp`

Array of particle z-coordinates for use with treecode routines

Definition at line 90 of file [vgreen.h](#).

The documentation for this struct was generated from the following file:

- [src/generic/vgreen.h](#)

8.22 sVgrid Struct Reference

Electrostatic potential oracle for Cartesian mesh data.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/mg/vgrid.h>
```

Data Fields

- int [nx](#)
- int [ny](#)
- int [nz](#)
- double [hx](#)
- double [hy](#)
- double [hz](#)
- double [xmin](#)
- double [ymin](#)
- double [zmin](#)
- double [xmax](#)
- double [ymax](#)
- double [zmax](#)
- double * [data](#)
- int [readdata](#)
- int [ctordata](#)
- Vmem * [mem](#)

8.22.1 Detailed Description

Electrostatic potential oracle for Cartesian mesh data.

Author

Nathan Baker

Definition at line [81](#) of file [vgrid.h](#).

8.22.2 Field Documentation

8.22.2.1 ctordata

int [ctordata](#)

flag indicating whether data was included at construction

Definition at line [97](#) of file [vgrid.h](#).

8.22.2.2 data

double* [data](#)

$nx \times ny \times nz$ array of data

Definition at line [95](#) of file [vgrid.h](#).

8.22.2.3 hx

double [hx](#)

Grid spacing in x direction

Definition at line [86](#) of file [vgrid.h](#).

8.22.2.4 hy

double [hy](#)

Grid spacing in y direction

Definition at line [87](#) of file [vgrid.h](#).

8.22.2.5 hzed

double hzed

Grid spacing in z direction

Definition at line 88 of file [vgrid.h](#).

8.22.2.6 mem

Vmem* mem

Memory manager object

Definition at line 99 of file [vgrid.h](#).

8.22.2.7 nx

int nx

Number grid points in x direction

Definition at line 83 of file [vgrid.h](#).

8.22.2.8 ny

int ny

Number grid points in y direction

Definition at line 84 of file [vgrid.h](#).

8.22.2.9 nz

int nz

Number grid points in z direction

Definition at line 85 of file [vgrid.h](#).

8.22.2.10 readdata

int readdata

flag indicating whether data was read from file

Definition at line 96 of file [vgrid.h](#).

8.22.2.11 xmax

double xmax

x coordinate of upper grid corner

Definition at line 92 of file [vgrid.h](#).

8.22.2.12 xmin

double xmin

x coordinate of lower grid corner

Definition at line 89 of file [vgrid.h](#).

8.22.2.13 ymax

double ymax

y coordinate of upper grid corner

Definition at line 93 of file [vgrid.h](#).

8.22.2.14 ymin

double ymin
 y coordinate of lower grid corner
 Definition at line 90 of file [vgrid.h](#).

8.22.2.15 zmax

double zmax
 z coordinate of upper grid corner
 Definition at line 94 of file [vgrid.h](#).

8.22.2.16 zmin

double zmin
 z coordinate of lower grid corner
 Definition at line 91 of file [vgrid.h](#).

The documentation for this struct was generated from the following file:

- [src/mg/vgrid.h](#)

8.23 sVmgrid Struct Reference

Multiresolution oracle for Cartesian mesh data.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/mg/vmgrid.h>
```

Data Fields

- int [ngrid](#)s
- [Vgrid](#) * [grids](#) [[VMGRIDMAX](#)]

8.23.1 Detailed Description

Multiresolution oracle for Cartesian mesh data.

Author

Nathan Baker

Definition at line 84 of file [vmgrid.h](#).

8.23.2 Field Documentation

8.23.2.1 grids

```
Vgrid* grids [VMGRIDMAX]
```

Grids in hierarchy. Our convention will be to have the finest grid first, however, this will not be enforced as it may be useful to search multiple grids for parallel datasets, etc.

Definition at line 87 of file [vmgrid.h](#).

8.23.2.2 ngrids

```
int ngrids
```

Number of grids in hierarchy

Definition at line 86 of file [vmgrid.h](#).

The documentation for this struct was generated from the following file:

- [src/mg/vmgrid.h](#)

8.24 sVopot Struct Reference

Electrostatic potential oracle for Cartesian mesh data.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/mg/vopot.h>
```

Data Fields

- `Vmgrid * mgrid`
- `Vpbe * pbe`
- `Vbcfl bcfl`

8.24.1 Detailed Description

Electrostatic potential oracle for Cartesian mesh data.

Author

Nathan Baker

Definition at line 83 of file [vopot.h](#).

8.24.2 Field Documentation

8.24.2.1 bcfl

`Vbcfl bcfl`

Boundary condition flag for returning potential values at points off the grid.

Definition at line 88 of file [vopot.h](#).

8.24.2.2 mgrid

`Vmgrid* mgrid`

Multiple grid object containing potential data (in units kT/e)

Definition at line 85 of file [vopot.h](#).

8.24.2.3 pbe

`Vpbe* pbe`

Pointer to PBE object

Definition at line 87 of file [vopot.h](#).

The documentation for this struct was generated from the following file:

- [src/mg/vopot.h](#)

8.25 sVparam_AtomData Struct Reference

AtomData sub-class; stores atom data.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/generic/vparam.h>
```

Data Fields

- char `atomName` [VMAX_ARGLEN]
- char `resName` [VMAX_ARGLEN]
- double `charge`
- double `radius`
- double `epsilon`

8.25.1 Detailed Description

AtomData sub-class; stores atom data.

Author

Nathan Baker

Note

The epsilon and radius members of this class refer use the following formula for calculating the van der Waals energy of atom i interacting with atom j :

$$V_{ij}(r_{ij}) = \epsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} - 2 \left(\frac{\sigma_{ij}}{r_{ij}} \right)^6 \right]$$

where $\epsilon_{ij} = \sqrt{\epsilon_i \epsilon_j}$ is the well-depth (in the desired energy units), r_{ij} is the distance between atoms i and j , and $\sigma_{ij} = \sigma_i + \sigma_j$ is the sum of the van der Waals radii.

Definition at line 92 of file [vparam.h](#).

8.25.2 Field Documentation

8.25.2.1 atomName

```
char atomName[VMAX_ARGLLEN]
```

Atom name

Definition at line 93 of file [vparam.h](#).

8.25.2.2 charge

```
double charge
```

Atom charge (in e)

Definition at line 95 of file [vparam.h](#).

8.25.2.3 epsilon

```
double epsilon
```

Atom VdW well depth (ϵ_i above; in kJ/mol)

Definition at line 97 of file [vparam.h](#).

8.25.2.4 radius

```
double radius
```

Atom VdW radius (σ_i above; in Å)

Definition at line 96 of file [vparam.h](#).

8.25.2.5 resName

```
char resName[VMAX_ARGLLEN]
```

Residue name

Definition at line 94 of file [vparam.h](#).

The documentation for this struct was generated from the following file:

- [src/generic/vparam.h](#)

8.26 sVpbe Struct Reference

Contains public data members for Vpbe class/module.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/generic/vpbe.h>
```

Data Fields

- Vmem * [vmem](#)
- [Valist](#) * [alist](#)
- [Vclist](#) * [clist](#)
- [Vacc](#) * [acc](#)
- double [T](#)
- double [soluteDiel](#)
- double [solventDiel](#)
- double [solventRadius](#)
- double [bulkIonicStrength](#)
- double [maxIonRadius](#)
- int [numIon](#)
- double [ionConc](#) [MAXION]
- double [ionRadii](#) [MAXION]
- double [ionQ](#) [MAXION]
- double [xkappa](#)
- double [deblen](#)
- double [zkappa2](#)
- double [zmagic](#)
- double [soluteCenter](#) [3]
- double [soluteRadius](#)
- double [soluteXlen](#)
- double [soluteYlen](#)
- double [soluteZlen](#)
- double [soluteCharge](#)
- double [smvolume](#)
- double [smsize](#)
- int [ipkey](#)
- int [paramFlag](#)
- double [z_mem](#)
- double [L](#)
- double [membraneDiel](#)
- double [V](#)
- int [param2Flag](#)

8.26.1 Detailed Description

Contains public data members for Vpbe class/module.

Author

Nathan Baker

Definition at line 84 of file [vpbe.h](#).

8.26.2 Field Documentation

8.26.2.1 acc

`Vacc* acc`

Accessibility object

Definition at line 90 of file [vpbe.h](#).

8.26.2.2 alist

`Valist* alist`

Atom (charge) list

Definition at line 88 of file [vpbe.h](#).

8.26.2.3 bulkIonicStrength

`double bulkIonicStrength`

Bulk ionic strength (M)

Definition at line 99 of file [vpbe.h](#).

8.26.2.4 clist

`Vclist* clist`

Atom location cell list

Definition at line 89 of file [vpbe.h](#).

8.26.2.5 deblen

`double deblen`

Debye length (bulk)

Definition at line 109 of file [vpbe.h](#).

8.26.2.6 ionConc

`double ionConc[MAXION]`

Concentration (M) of each species

Definition at line 104 of file [vpbe.h](#).

8.26.2.7 ionQ

`double ionQ[MAXION]`

Charge (e) of each species

Definition at line 106 of file [vpbe.h](#).

8.26.2.8 ionRadii

`double ionRadii[MAXION]`

Ionic radius (Å) of each species

Definition at line 105 of file [vpbe.h](#).

8.26.2.9 ipkey

`int ipkey`

PBE calculation type (this is a cached copy it should not be used directly in code)

Definition at line 122 of file [vpbe.h](#).

8.26.2.10 L

```
double L
```

Length of the membrane (A)

Definition at line 132 of file [vpbe.h](#).

8.26.2.11 maxIonRadius

```
double maxIonRadius
```

Max ion radius (A; used for calculating accessibility and defining volumes for ionic strength coefficients)

Definition at line 100 of file [vpbe.h](#).

8.26.2.12 membraneDiel

```
double membraneDiel
```

Membrane dielectric constant

Definition at line 133 of file [vpbe.h](#).

8.26.2.13 numIon

```
int numIon
```

Total number of ion species

Definition at line 103 of file [vpbe.h](#).

8.26.2.14 param2Flag

```
int param2Flag
```

Check to see if bcfl=3 parms have been set

Definition at line 135 of file [vpbe.h](#).

8.26.2.15 paramFlag

```
int paramFlag
```

Check to see if the parameters have been set

Definition at line 125 of file [vpbe.h](#).

8.26.2.16 smsize

```
double smsize
```

Size-Modified PBE size

Definition at line 121 of file [vpbe.h](#).

8.26.2.17 smvolume

```
double smvolume
```

Size-Modified PBE relative volume

Definition at line 120 of file [vpbe.h](#).

8.26.2.18 soluteCenter

```
double soluteCenter[3]
```

Center of solute molecule (A)

Definition at line 113 of file [vpbe.h](#).

8.26.2.19 soluteCharge

```
double soluteCharge
```

Charge of solute molecule (e)

Definition at line 118 of file [vpbe.h](#).

8.26.2.20 soluteDiel

```
double soluteDiel
```

Solute dielectric constant (unitless)

Definition at line 93 of file [vpbe.h](#).

8.26.2.21 soluteRadius

```
double soluteRadius
```

Radius of solute molecule (A)

Definition at line 114 of file [vpbe.h](#).

8.26.2.22 soluteXlen

```
double soluteXlen
```

Solute length in x-direction

Definition at line 115 of file [vpbe.h](#).

8.26.2.23 soluteYlen

```
double soluteYlen
```

Solute length in y-direction

Definition at line 116 of file [vpbe.h](#).

8.26.2.24 soluteZlen

```
double soluteZlen
```

Solute length in z-direction

Definition at line 117 of file [vpbe.h](#).

8.26.2.25 solventDiel

```
double solventDiel
```

Solvent dielectric constant (unitless)

Definition at line 94 of file [vpbe.h](#).

8.26.2.26 solventRadius

```
double solventRadius
```

Solvent probe radius (angstroms) for accessibility; determining defining volumes for the dielectric coefficient

Definition at line 95 of file [vpbe.h](#).

8.26.2.27 T

```
double T
```

Temperature (K)

Definition at line 92 of file [vpbe.h](#).

8.26.2.28 V`double V`

Membrane potential

Definition at line 134 of file [vpbe.h](#).**8.26.2.29 vmem**`Vmem* vmem`

Memory management object

Definition at line 86 of file [vpbe.h](#).**8.26.2.30 xkappa**`double xkappa`

Debye-Huckel parameter (bulk)

Definition at line 108 of file [vpbe.h](#).**8.26.2.31 z_mem**`double z_mem`

Z value of the bottom of the membrane (A)

Definition at line 131 of file [vpbe.h](#).**8.26.2.32 zkappa2**`double zkappa2`

Square of modified Debye-Huckel parameter (bulk)

Definition at line 110 of file [vpbe.h](#).**8.26.2.33 zmagic**`double zmagic`

Delta function scaling parameter

Definition at line 111 of file [vpbe.h](#).

The documentation for this struct was generated from the following file:

- [src/generic/vpbe.h](#)

8.27 sVpee Struct Reference

Contains public data members for Vpee class/module.

`#include </builddir/build/BUILD/apbs-3.0.0/src/fem/vpee.h>`**Data Fields**

- Gem * [gm](#)
- int [localPartID](#)
- double [localPartCenter](#) [3]
- double [localPartRadius](#)
- int [killFlag](#)
- double [killParam](#)
- Vmem * [mem](#)

8.27.1 Detailed Description

Contains public data members for Vpee class/module.

Author

Nathan Baker

Definition at line 89 of file [vpee.h](#).

8.27.2 Field Documentation

8.27.2.1 gm

`Gem* gm`

Grid manager

Definition at line 91 of file [vpee.h](#).

8.27.2.2 killFlag

`int killFlag`

A flag indicating the method we're using to artificially decrease the error estimate outside the local partition

Definition at line 99 of file [vpee.h](#).

8.27.2.3 killParam

`double killParam`

A parameter for the error estimate attenuation method

Definition at line 102 of file [vpee.h](#).

8.27.2.4 localPartCenter

`double localPartCenter[3]`

The coordinates of the center of the local partition

Definition at line 95 of file [vpee.h](#).

8.27.2.5 localPartID

`int localPartID`

The local partition ID: i.e. the partition whose boundary simplices we're keeping track of

Definition at line 92 of file [vpee.h](#).

8.27.2.6 localPartRadius

`double localPartRadius`

The radius of the circle/sphere which circumscribes the local partition

Definition at line 97 of file [vpee.h](#).

8.27.2.7 mem

`Vmem* mem`

Memory manager

Definition at line 104 of file [vpee.h](#).

The documentation for this struct was generated from the following file:

- [src/fem/vpee.h](#)

8.28 sVpmg Struct Reference

Contains public data members for Vpmg class/module.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/mg/vpmg.h>
```

Data Fields

- Vmem * [vmem](#)
- [Vpmgp](#) * [pmgp](#)
- [Vpbe](#) * [pbe](#)
- double * [epsx](#)
- double * [epsy](#)
- double * [epsz](#)
- double * [kappa](#)
- double * [pot](#)
- double * [charge](#)
- int * [iparm](#)
- double * [rparm](#)
- int * [iwork](#)
- double * [rwork](#)
- double * [a1cf](#)
- double * [a2cf](#)
- double * [a3cf](#)
- double * [ccf](#)
- double * [fcf](#)
- double * [tcf](#)
- double * [u](#)
- double * [xf](#)
- double * [yf](#)
- double * [zf](#)
- double * [gxcf](#)
- double * [gycf](#)
- double * [gzcf](#)
- double * [pvec](#)
- double [extDiEnergy](#)
- double [extQmEnergy](#)
- double [extQfEnergy](#)
- double [extNpEnergy](#)
- Vsurf_Meth [surfMeth](#)
- double [splineWin](#)
- Vchrg_Meth [chargeMeth](#)
- Vchrg_Src [chargeSrc](#)
- int [filled](#)
- int [useDielXMap](#)
- [Vgrid](#) * [dielXMap](#)
- int [useDielYMap](#)
- [Vgrid](#) * [dielYMap](#)
- int [useDielZMap](#)
- [Vgrid](#) * [dielZMap](#)
- int [useKappaMap](#)
- [Vgrid](#) * [kappaMap](#)

- int [usePotMap](#)
- [Vgrid](#) * [potMap](#)
- int [useChargeMap](#)
- [Vgrid](#) * [chargeMap](#)

8.28.1 Detailed Description

Contains public data members for Vpmg class/module.

Author

Nathan Baker

Many of the routines and macros are borrowed from the [main.c](#) driver (written by Mike Holst) provided with the PMG code.

Definition at line [116](#) of file [vpmg.h](#).

8.28.2 Field Documentation

8.28.2.1 a1cf

`double* a1cf`

Operator coefficient values (a11) – this array can be overwritten

Definition at line [138](#) of file [vpmg.h](#).

8.28.2.2 a2cf

`double* a2cf`

Operator coefficient values (a22) – this array can be overwritten

Definition at line [140](#) of file [vpmg.h](#).

8.28.2.3 a3cf

`double* a3cf`

Operator coefficient values (a33) – this array can be overwritten

Definition at line [142](#) of file [vpmg.h](#).

8.28.2.4 ccf

`double* ccf`

Helmholtz term – this array can be overwritten

Definition at line [144](#) of file [vpmg.h](#).

8.28.2.5 charge

`double* charge`

Charge map

Definition at line [132](#) of file [vpmg.h](#).

8.28.2.6 chargeMap

[Vgrid](#)* [chargeMap](#)

External charge distribution map

Definition at line [188](#) of file [vpmg.h](#).

8.28.2.7 chargeMeth

Vchrg_Meth chargeMeth

Charge discretization method

Definition at line 165 of file [vpmpg.h](#).

8.28.2.8 chargeSrc

Vchrg_Src chargeSrc

Charge source

Definition at line 166 of file [vpmpg.h](#).

8.28.2.9 dielXMap

Vgrid* dielXMap

External x-shifted dielectric map

Definition at line 172 of file [vpmpg.h](#).

8.28.2.10 dielYMap

Vgrid* dielYMap

External y-shifted dielectric map

Definition at line 175 of file [vpmpg.h](#).

8.28.2.11 dielZMap

Vgrid* dielZMap

External z-shifted dielectric map

Definition at line 178 of file [vpmpg.h](#).

8.28.2.12 epsx

double* epsx

X-shifted dielectric map

Definition at line 127 of file [vpmpg.h](#).

8.28.2.13 epsy

double* epsy

Y-shifted dielectric map

Definition at line 128 of file [vpmpg.h](#).

8.28.2.14 epsz

double* epsz

Y-shifted dielectric map

Definition at line 129 of file [vpmpg.h](#).

8.28.2.15 extDiEnergy

double extDiEnergy

Stores contributions to the dielectric energy from regions outside the problem domain

Definition at line 155 of file [vpmpg.h](#).

8.28.2.16 extNpEnergy

`double extNpEnergy`

Stores contributions to the apolar energy from regions outside the problem domain

Definition at line 161 of file [vpmg.h](#).

8.28.2.17 extQfEnergy

`double extQfEnergy`

Stores contributions to the fixed charge energy from regions outside the problem domain

Definition at line 159 of file [vpmg.h](#).

8.28.2.18 extQmEnergy

`double extQmEnergy`

Stores contributions to the mobile ion energy from regions outside the problem domain

Definition at line 157 of file [vpmg.h](#).

8.28.2.19 fcf

`double* fcf`

Right-hand side – this array can be overwritten

Definition at line 145 of file [vpmg.h](#).

8.28.2.20 filled

`int filled`

Indicates whether `Vpmg_fillco` has been called

Definition at line 168 of file [vpmg.h](#).

8.28.2.21 gxcf

`double* gxcf`

Boundary conditions for x faces

Definition at line 151 of file [vpmg.h](#).

8.28.2.22 gyxf

`double* gyxf`

Boundary conditions for y faces

Definition at line 152 of file [vpmg.h](#).

8.28.2.23 gzcf

`double* gzcf`

Boundary conditions for z faces

Definition at line 153 of file [vpmg.h](#).

8.28.2.24 iparm

`int* iparm`

Passing int parameters to FORTRAN

Definition at line 134 of file [vpmg.h](#).

8.28.2.25 iwork

```
int* iwork
```

Work array

Definition at line 136 of file [vpmg.h](#).

8.28.2.26 kappa

```
double* kappa
```

Ion accessibility map ($0 \leq \text{kappa}(x) \leq 1$)

Definition at line 130 of file [vpmg.h](#).

8.28.2.27 kappaMap

```
Vgrid* kappaMap
```

External kappa map

Definition at line 181 of file [vpmg.h](#).

8.28.2.28 pbe

```
Vpbe* pbe
```

Information about the PBE system

Definition at line 120 of file [vpmg.h](#).

8.28.2.29 pmgp

```
Vpmgp* pmgp
```

Parameters

Definition at line 119 of file [vpmg.h](#).

8.28.2.30 pot

```
double* pot
```

Potential map

Definition at line 131 of file [vpmg.h](#).

8.28.2.31 potMap

```
Vgrid* potMap
```

External potential map

Definition at line 184 of file [vpmg.h](#).

8.28.2.32 pvec

```
double* pvec
```

Partition mask array

Definition at line 154 of file [vpmg.h](#).

8.28.2.33 rparm

```
double* rparm
```

Passing real parameters to FORTRAN

Definition at line 135 of file [vpmg.h](#).

8.28.2.34 **rwork**

`double* rwork`

Work array

Definition at line 137 of file [vpmg.h](#).

8.28.2.35 **splineWin**

`double splineWin`

Spline window parm for surf defs

Definition at line 164 of file [vpmg.h](#).

8.28.2.36 **surfMeth**

`Vsurf_Meth surfMeth`

Surface definition method

Definition at line 163 of file [vpmg.h](#).

8.28.2.37 **tcf**

`double* tcf`

True solution

Definition at line 146 of file [vpmg.h](#).

8.28.2.38 **u**

`double* u`

Solution

Definition at line 147 of file [vpmg.h](#).

8.28.2.39 **useChargeMap**

`int useChargeMap`

Indicates whether Vpmg_fillco was called with an external charge distribution map

Definition at line 186 of file [vpmg.h](#).

8.28.2.40 **useDielXMap**

`int useDielXMap`

Indicates whether Vpmg_fillco was called with an external x-shifted dielectric map

Definition at line 170 of file [vpmg.h](#).

8.28.2.41 **useDielYMap**

`int useDielYMap`

Indicates whether Vpmg_fillco was called with an external y-shifted dielectric map

Definition at line 173 of file [vpmg.h](#).

8.28.2.42 **useDielZMap**

`int useDielZMap`

Indicates whether Vpmg_fillco was called with an external z-shifted dielectric map

Definition at line 176 of file [vpmg.h](#).

8.28.2.43 useKappaMap

int useKappaMap

Indicates whether Vpmg_fillco was called with an external kappa map

Definition at line 179 of file [vpmg.h](#).

8.28.2.44 usePotMap

int usePotMap

Indicates whether Vpmg_fillco was called with an external potential map

Definition at line 182 of file [vpmg.h](#).

8.28.2.45 vmem

Vmem* vmem

Memory management object for this class

Definition at line 118 of file [vpmg.h](#).

8.28.2.46 xf

double* xf

Mesh point x coordinates

Definition at line 148 of file [vpmg.h](#).

8.28.2.47 yf

double* yf

Mesh point y coordinates

Definition at line 149 of file [vpmg.h](#).

8.28.2.48 zf

double* zf

Mesh point z coordinates

Definition at line 150 of file [vpmg.h](#).

The documentation for this struct was generated from the following file:

- [src/mg/vpmg.h](#)

8.29 sVpmgp Struct Reference

Contains public data members for Vpmgp class/module.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/mg/vpmgp.h>
```

Data Fields

- int [nx](#)
- int [ny](#)
- int [nz](#)
- int [nlev](#)
- double [hx](#)
- double [hy](#)
- double [hz](#)
- int [nonlin](#)

- int [nxc](#)
- int [nyc](#)
- int [nzc](#)
- int [nf](#)
- int [nc](#)
- int [narrc](#)
- int [n_rpc](#)
- int [n_iz](#)
- int [n_ipc](#)
- size_t [nrwk](#)
- int [niwk](#)
- int [narr](#)
- int [ipkey](#)
- double [xcent](#)
- double [ycent](#)
- double [zcent](#)
- double [errtol](#)
- int [itmax](#)
- int [istop](#)
- int [iinfo](#)
- [Vbcfl](#) [bcfl](#)
- int [key](#)
- int [iperf](#)
- int [meth](#)
- int [mgkey](#)
- int [nu1](#)
- int [nu2](#)
- int [mgsmoo](#)
- int [mgprol](#)
- int [mgcoar](#)
- int [mgsolv](#)
- int [mgdisc](#)
- double [omegal](#)
- double [omegan](#)
- int [irite](#)
- int [ipcon](#)
- double [xlen](#)
- double [ylen](#)
- double [zlen](#)
- double [xmin](#)
- double [ymin](#)
- double [zmin](#)
- double [xmax](#)
- double [ymax](#)
- double [zmax](#)

8.29.1 Detailed Description

Contains public data members for Vpmgp class/module.

Author

Nathan Baker

Bug Value ipcon does not currently allow for preconditioning in PMG

Definition at line 80 of file [vpmgp.h](#).

8.29.2 Field Documentation

8.29.2.1 bcfl

`Vbcfl bcfl`

Boundary condition method [default = BCFL_SDH]

Definition at line 135 of file [vpmgp.h](#).

8.29.2.2 errtol

`double errtol`

Desired error tolerance [default = 1e-9]

Definition at line 121 of file [vpmgp.h](#).

8.29.2.3 hx

`double hx`

Grid x spacings [no default]

Definition at line 87 of file [vpmgp.h](#).

8.29.2.4 hy

`double hy`

Grid y spacings [no default]

Definition at line 88 of file [vpmgp.h](#).

8.29.2.5 hzed

`double hzed`

Grid z spacings [no default]

Definition at line 89 of file [vpmgp.h](#).

8.29.2.6 iinfo

`int iinfo`

Runtime status messages [default = 1]

- 0: none
- 1: some
- 2: lots
- 3: more

Definition at line 130 of file [vpmgp.h](#).

8.29.2.7 ipcon

`int ipcon`

Preconditioning method [default = 3]

- 0: diagonal
- 1: ICCG
- 2: ICCGDW
- 3: MICCGDW
- 4: none

Definition at line 183 of file [vpmgp.h](#).

8.29.2.8 iperf

`int iperf`

Analysis of the operator [default = 0]

- 0: no
- 1: condition number
- 2: spectral radius
- 3: cond. number & spectral radius

Definition at line 139 of file [vpmgp.h](#).

8.29.2.9 ipkey

`int ipkey`

Toggles nonlinearity (set by `nonlin`)

- -2: Size-Modified PBE
- -1: Linearized PBE
- 0: Nonlinear PBE with capped sinh term [default]
- >1: Polynomial approximation to sinh, note that `ipkey` must be odd

Definition at line 109 of file [vpmgp.h](#).

8.29.2.10 irite

`int irite`

FORTTRAN output unit [default = 8]

Definition at line 182 of file [vpmgp.h](#).

8.29.2.11 istop

```
int istop
```

Stopping criterion [default = 1]

- 0: residual
- 1: relative residual
- 2: diff
- 3: errc
- 4: errd
- 5: aerrd

Definition at line 123 of file [vpmgp.h](#).

8.29.2.12 itmax

```
int itmax
```

Maximum number of iters [default = 100]

Definition at line 122 of file [vpmgp.h](#).

8.29.2.13 key

```
int key
```

Print solution to file [default = 0]

- 0: no
- 1: yes

Definition at line 136 of file [vpmgp.h](#).

8.29.2.14 meth

```
int meth
```

Solution method [default = 2]

- 0: conjugate gradient multigrid
- 1: newton
- 2: multigrid
- 3: conjugate gradient
- 4: successive overrelaxation
- 5: red-black gauss-seidel
- 6: weighted jacobi
- 7: richardson
- 8: conjugate gradient multigrid aqua
- 9: newton aqua

Definition at line 144 of file [vpmgp.h](#).

8.29.2.15 mgcoar

`int mgcoar`

Coarsening method [default = 2]

- 0: standard
- 1: harmonic
- 2: galerkin

Definition at line 170 of file [vpmgp.h](#).

8.29.2.16 mgdisc

`int mgdisc`

Discretization method [default = 0]

- 0: finite volume
- 1: finite element

Definition at line 177 of file [vpmgp.h](#).

8.29.2.17 mgkey

`int mgkey`

Multigrid method [default = 0]

- 0: variable v-cycle
- 1: nested iteration

Definition at line 155 of file [vpmgp.h](#).

8.29.2.18 mgprol

`int mgprol`

Prolongation method [default = 0]

- 0: trilinear
- 1: operator-based
- 2: mod. operator-based

Definition at line 166 of file [vpmgp.h](#).

8.29.2.19 mgsmoo

`int mgsmoo`

Smoothing method [default = 1]

- 0: weighted jacobi
- 1: gauss-seidel
- 2: SOR
- 3: richardson
- 4: cghs

Definition at line 160 of file [vpmgp.h](#).

8.29.2.20 mgsolv

```
int mgsolv
```

Coarse equation solve method [default = 1]

- 0: cghs
- 1: banded linpack

Definition at line 174 of file [vpmgp.h](#).

8.29.2.21 n_ipc

```
int n_ipc
```

Integer info work array required storage

Definition at line 104 of file [vpmgp.h](#).

8.29.2.22 n_iz

```
int n_iz
```

Integer storage parameter (index max)

Definition at line 103 of file [vpmgp.h](#).

8.29.2.23 n_rpc

```
int n_rpc
```

Real info work array required storage

Definition at line 102 of file [vpmgp.h](#).

8.29.2.24 narr

```
int narr
```

Array work storage

Definition at line 108 of file [vpmgp.h](#).

8.29.2.25 narrc

```
int narrc
```

Size of vector on coarse level

Definition at line 101 of file [vpmgp.h](#).

8.29.2.26 nc

```
int nc
```

Number of coarse grid unknowns

Definition at line 100 of file [vpmgp.h](#).

8.29.2.27 nf

```
int nf
```

Number of fine grid unknowns

Definition at line 99 of file [vpmgp.h](#).

8.29.2.28 niwk

```
int niwk
```

Integer work storage

Definition at line 107 of file [vpmgp.h](#).

8.29.2.29 nlev

```
int nlev
```

Number of mesh levels [no default]

Definition at line 86 of file [vpmgp.h](#).

8.29.2.30 nonlin

```
int nonlin
```

Problem type [no default]

- 0: linear
- 1: nonlinear
- 2: linear then nonlinear

Definition at line 90 of file [vpmgp.h](#).

8.29.2.31 nrwk

```
size_t nrwk
```

Real work storage

Definition at line 106 of file [vpmgp.h](#).

8.29.2.32 nu1

```
int nul
```

Number of pre-smoothings [default = 2]

Definition at line 158 of file [vpmgp.h](#).

8.29.2.33 nu2

```
int nu2
```

Number of post-smoothings [default = 2]

Definition at line 159 of file [vpmgp.h](#).

8.29.2.34 nx

```
int nx
```

Grid x dimensions [no default]

Definition at line 83 of file [vpmgp.h](#).

8.29.2.35 nxc

```
int nxc
```

Coarse level grid x dimensions

Definition at line 96 of file [vpmgp.h](#).

8.29.2.36 ny

```
int ny
```

Grid y dimensions [no default]

Definition at line 84 of file [vpmgp.h](#).

8.29.2.37 nyc

```
int nyc
```

Coarse level grid y dimensions

Definition at line 97 of file [vpmgp.h](#).

8.29.2.38 nz

```
int nz
```

Grid z dimensions [no default]

Definition at line 85 of file [vpmgp.h](#).

8.29.2.39 nzc

```
int nzc
```

Coarse level grid z dimensions

Definition at line 98 of file [vpmgp.h](#).

8.29.2.40 omegal

```
double omegal
```

Linear relax parameter [default = 8e-1]

Definition at line 180 of file [vpmgp.h](#).

8.29.2.41 omegan

```
double omegan
```

Nonlin relax parameter [default = 9e-1]

Definition at line 181 of file [vpmgp.h](#).

8.29.2.42 xcent

```
double xcent
```

Grid x center [0]

Definition at line 118 of file [vpmgp.h](#).

8.29.2.43 xlen

```
double xlen
```

Domain x length

Definition at line 189 of file [vpmgp.h](#).

8.29.2.44 xmax

```
double xmax
```

Domain upper x corner

Definition at line 195 of file [vpmgp.h](#).

8.29.2.45 xmin

```
double xmin
```

Domain lower x corner

Definition at line 192 of file [vpmgp.h](#).

8.29.2.46 ycent

double ycent
Grid y center [0]

Definition at line 119 of file [vpmgp.h](#).

8.29.2.47 ylen

double ylen
Domain y length
Definition at line 190 of file [vpmgp.h](#).

8.29.2.48 ymax

double ymax
Domain upper y corner
Definition at line 196 of file [vpmgp.h](#).

8.29.2.49 ymin

double ymin
Domain lower y corner
Definition at line 193 of file [vpmgp.h](#).

8.29.2.50 zcent

double zcent
Grid z center [0]

Definition at line 120 of file [vpmgp.h](#).

8.29.2.51 zlen

double zlen
Domain z length
Definition at line 191 of file [vpmgp.h](#).

8.29.2.52 zmax

double zmax
Domain upper z corner
Definition at line 197 of file [vpmgp.h](#).

8.29.2.53 zmin

double zmin
Domain lower z corner
Definition at line 194 of file [vpmgp.h](#).

The documentation for this struct was generated from the following file:

- [src/mg/vpmgp.h](#)

8.30 Vparam Struct Reference

Reads and assigns charge/radii parameters.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/generic/vparam.h>
```

Data Fields

- Vmem * [vmem](#)
- int [nResData](#)
- [Vparam_ResData](#) * [resData](#)

8.30.1 Detailed Description

Reads and assigns charge/radii parameters.

Author

Nathan Baker

Definition at line [135](#) of file [vparam.h](#).

8.30.2 Field Documentation

8.30.2.1 nResData

```
int nResData
```

Number of [Vparam_ResData](#) objects associated with this object

Definition at line [138](#) of file [vparam.h](#).

8.30.2.2 resData

```
Vparam_ResData* resData
```

Array of nResData [Vparam_ResData](#) objects

Definition at line [140](#) of file [vparam.h](#).

8.30.2.3 vmem

```
Vmem* vmem
```

Memory management object for this class

Definition at line [137](#) of file [vparam.h](#).

The documentation for this struct was generated from the following file:

- [src/generic/vparam.h](#)

8.31 Vparam_ResData Struct Reference

ResData sub-class; stores residue data.

```
#include </builddir/build/BUILD/apbs-3.0.0/src/generic/vparam.h>
```

Data Fields

- Vmem * [vmem](#)
- char [name](#) [VMAX_ARGLEN]
- int [nAtomData](#)
- [Vparam_AtomData](#) * [atomData](#)

8.31.1 Detailed Description

ResData sub-class; stores residue data.

Author

Nathan Baker

Definition at line 114 of file [vparam.h](#).

8.31.2 Field Documentation

8.31.2.1 atomData

[Vparam_AtomData](#)* atomData

Array of [Vparam_AtomData](#) natom objects

Definition at line 119 of file [vparam.h](#).

8.31.2.2 name

char name[VMAX_ARGLEN]

Residue name

Definition at line 116 of file [vparam.h](#).

8.31.2.3 nAtomData

int nAtomData

Number of [Vparam_AtomData](#) objects associated with this object

Definition at line 117 of file [vparam.h](#).

8.31.2.4 vmem

Vmem* vmem

Pointer to memory manager from [Vparam](#) master class

Definition at line 115 of file [vparam.h](#).

The documentation for this struct was generated from the following file:

- [src/generic/vparam.h](#)

Chapter 9

File Documentation

9.1 mainpage.h

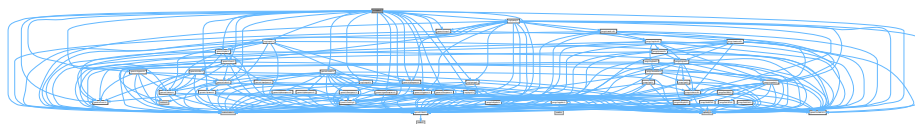
00001

9.2 src/apbs.h File Reference

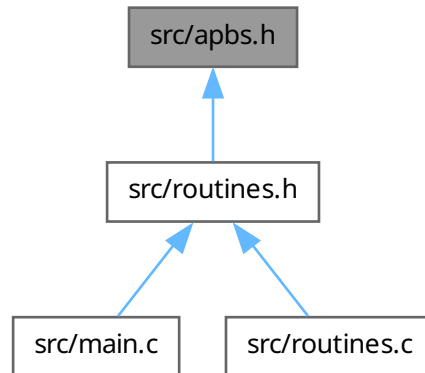
Header file for header dependencies.

```
#include "apbscfg.h"
#include "malloc/malloc.h"
#include "generic/nosh.h"
#include "generic/mgparm.h"
#include "generic/pbeparm.h"
#include "generic/femparm.h"
#include "generic/bemparm.h"
#include "generic/geoflowparm.h"
#include "generic/vacc.h"
#include "generic/valist.h"
#include "generic/vatom.h"
#include "generic/vcap.h"
#include "generic/vhal.h"
#include "generic/vpbe.h"
#include "generic/vstring.h"
#include "generic/vunit.h"
#include "generic/vparam.h"
#include "generic/vgreen.h"
#include "mg/vgrid.h"
#include "mg/vmgrid.h"
#include "mg/vopot.h"
#include "mg/vpmg.h"
#include "mg/vpmgp.h"
```

Include dependency graph for apbs.h:



This graph shows which files directly or indirectly include this file:



9.2.1 Detailed Description

Header file for header dependencies.

Author

Nathan Baker

Version

\$Id\$

Attention

```

*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
* Nathan A. Baker (nathan.baker@pnnl.gov)
* Pacific Northwest National Laboratory
*
* Additional contributing authors listed in the code documentation.
*
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```

```

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* ARISING IN ANY WAY OUT OF THE USE OF THIS SOFTWARE, EVEN IF ADVISED OF
* THE POSSIBILITY OF SUCH DAMAGE.
*
*

```

Definition in file [apbs.h](#).

9.3 apbs.h

[Go to the documentation of this file.](#)

```

00001
00061 #ifndef _APBSHEADERS_H_
00062 #define _APBSHEADERS_H_
00063
00064 #include "apbscfg.h"
00065
00066 /* MALLOC headers */
00067 #include "malloc/malloc.h"
00068
00069 /* Generic headers */
00070 #include "generic/nosh.h"
00071 #include "generic/mgparm.h"
00072 #include "generic/pbeparm.h"
00073 #include "generic/femparm.h"
00074 #include "generic/bemparm.h"
00075 #include "generic/geoflowparm.h"
00076 #include "generic/vacc.h"
00077 #include "generic/valist.h"
00078 #include "generic/vatom.h"
00079 #include "generic/vcap.h"
00080 #include "generic/vhal.h"
00081 #include "generic/vpbe.h"
00082 #include "generic/vstring.h"
00083 #include "generic/vunit.h"
00084 #include "generic/vparam.h"
00085 #include "generic/vgreen.h"
00086
00087 // #include "geoflow/cpbconcz2.h"
00088
00089 /* MG headers */
00090 #include "mg/vgrid.h"
00091 #include "mg/vmgrid.h"
00092 #include "mg/vopot.h"
00093 #include "mg/vpmg.h"
00094 #include "mg/vpmgp.h"
00095
00096 /* FEM headers */
00097 #if defined(FETK_ENABLED)
00098     #include "fem/vfetc.h"
00099     #include "fem/vpee.h"
00100 #endif
00101
00102 #endif /* _APBSHEADERS_H_ */

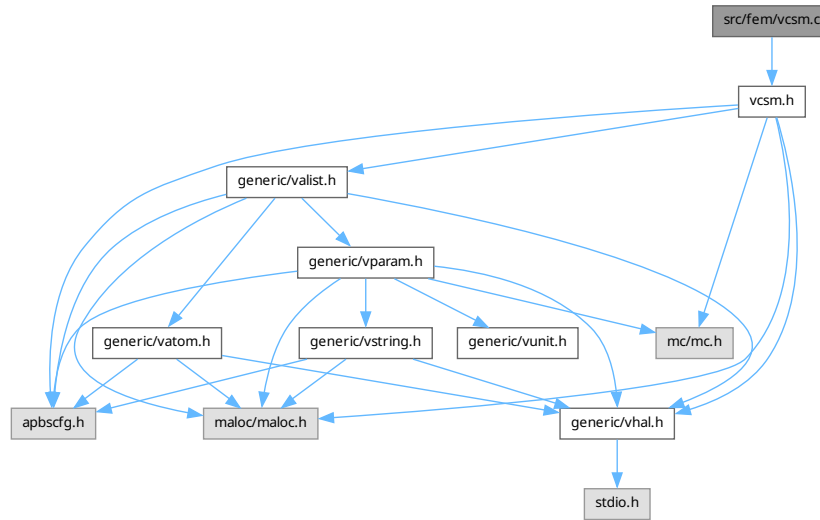
```

9.4 src/fem/vcsm.c File Reference

Class Vcsm methods.

```
#include "vcsm.h"
```

Include dependency graph for vcsm.c:



Functions

- VPUBLIC Valist * Vcsm_getValist (Vcsm *thee)
Get atom list.
- VPUBLIC int Vcsm_getNumberAtoms (Vcsm *thee, int isimp)
Get number of atoms associated with a simplex.
- VPUBLIC Vatom * Vcsm_getAtom (Vcsm *thee, int iatom, int isimp)
Get particular atom associated with a simplex.
- VPUBLIC int Vcsm_getAtomIndex (Vcsm *thee, int iatom, int isimp)
Get ID of particular atom in a simplex.
- VPUBLIC int Vcsm_getNumberSimplexes (Vcsm *thee, int iatom)
Get number of simplexes associated with an atom.
- VPUBLIC SS * Vcsm_getSimplex (Vcsm *thee, int isimp, int iatom)
Get particular simplex associated with an atom.
- VPUBLIC int Vcsm_getSimplexIndex (Vcsm *thee, int isimp, int iatom)
Get index particular simplex associated with an atom.
- VPUBLIC unsigned long int Vcsm_memChk (Vcsm *thee)
Return the memory used by this structure (and its contents) in bytes.
- VPUBLIC Vcsm * Vcsm_ctor (Valist *alist, Gem *gm)
Construct Vcsm object.
- VPUBLIC int Vcsm_ctor2 (Vcsm *thee, Valist *alist, Gem *gm)
FORTTRAN stub to construct Vcsm object.
- VPUBLIC void Vcsm_init (Vcsm *thee)
Initialize charge-simplex map with mesh and atom data.

- VPUBLIC void `Vcsm_dtor` (`Vcsm **thee`)
Destroy Vcsm object.
- VPUBLIC void `Vcsm_dtor2` (`Vcsm *thee`)
FORTTRAN stub to destroy Vcsm object.
- VPUBLIC int `Vcsm_update` (`Vcsm *thee`, SS `**simps`, int num)
Update the charge-simplex and simplex-charge maps after refinement.

9.4.1 Detailed Description

Class Vcsm methods.

Author

Nathan Baker

Version

\$Id\$

Attention

```
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* APBS -- Adaptive Poisson-Boltzmann Solver
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```

```

* THE POSSIBILITY OF SUCH DAMAGE.
*
*

```

Definition in file [vcsn.c](#).

9.5 vcsn.c

[Go to the documentation of this file.](#)

```

00001
00057 #include "vcsn.h"
00058
00059 /* Inlineable methods */
00060 #if !defined(VINLINE_VCSM)
00061
00062 VPUBLIC Valist* Vcsn_getValist(Vcsn *thee) {
00063     VASSERT(thee != VNULL);
00064     return thee->alist;
00065 }
00066
00067
00068
00069 VPUBLIC int Vcsn_getNumberAtoms(Vcsn *thee, int isimp) {
00070
00071     VASSERT(thee != VNULL);
00072     VASSERT(thee->initFlag);
00073     return thee->nsqm[isimp];
00074 }
00075
00076
00077 VPUBLIC Vatom* Vcsn_getAtom(Vcsn *thee, int iatom, int isimp) {
00078
00079     VASSERT(thee != VNULL);
00080     VASSERT(thee->initFlag);
00081
00082     VASSERT(iatom < (thee->nsqm)[isimp]);
00083     return Valist_getAtom(thee->alist, (thee->sqm)[isimp][iatom]);
00084 }
00085
00086
00087
00088 VPUBLIC int Vcsn_getAtomIndex(Vcsn *thee, int iatom, int isimp) {
00089
00090     VASSERT(thee != VNULL);
00091     VASSERT(thee->initFlag);
00092
00093     VASSERT(iatom < (thee->nsqm)[isimp]);
00094     return (thee->sqm)[isimp][iatom];
00095 }
00096
00097
00098
00099 VPUBLIC int Vcsn_getNumberSimplices(Vcsn *thee, int iatom) {
00100
00101     VASSERT(thee != VNULL);
00102     VASSERT(thee->initFlag);
00103
00104     return (thee->nqsm)[iatom];
00105 }
00106
00107
00108
00109 VPUBLIC SS* Vcsn_getSimplex(Vcsn *thee, int isimp, int iatom) {
00110
00111     VASSERT(thee != VNULL);
00112     VASSERT(thee->initFlag);
00113
00114     return Gem_SS(thee->gm, (thee->qsm)[iatom][isimp]);
00115 }
00116
00117
00118
00119 VPUBLIC int Vcsn_getSimplexIndex(Vcsn *thee, int isimp, int iatom) {
00120
00121     VASSERT(thee != VNULL);
00122     VASSERT(thee->initFlag);
00123

```



```

00124
00125     return (thee->qsm)[iatom][isimp];
00126
00127 }
00128
00129 VPUBLIC unsigned long int Vcsn_memChk(Vcsn *thee) {
00130     if (thee == VNULL) return 0;
00131     return Vmem_bytes(thee->vmem);
00132 }
00133
00134 #endif /* if !defined(VINLINE_VCSM) */
00135
00136 VPUBLIC Vcsn* Vcsn_ctor(Valist *alist, Gem *gm) {
00137
00138     /* Set up the structure */
00139     Vcsn *thee = VNULL;
00140     thee = (Vcsn*)Vmem_malloc(VNULL, 1, sizeof(Vcsn) );
00141     VASSERT( thee != VNULL);
00142     VASSERT( Vcsn_ctor2(thee, alist, gm));
00143
00144     return thee;
00145 }
00146
00147 VPUBLIC int Vcsn_ctor2(Vcsn *thee, Valist *alist, Gem *gm) {
00148     VASSERT( thee != VNULL );
00149
00150     /* Memory management object */
00151     thee->vmem = Vmem_ctor("APBS:VCSM");
00152
00153     /* Set up the atom list and grid manager */
00154     if( alist == VNULL) {
00155         Vnm_print(2, "Vcsn_ctor2: got null pointer to Valist object!\n");
00156         return 0;
00157     }
00158     thee->alist = alist;
00159     if( gm == VNULL) {
00160         Vnm_print(2, "Vcsn_ctor2: got a null pointer to the Gem object!\n");
00161         return 0;
00162     }
00163     thee->gm = gm;
00164
00165     thee->initFlag = 0;
00166     return 1;
00167 }
00168
00169
00170 VPUBLIC void Vcsn_init(Vcsn *thee) {
00171
00172     /* Counters */
00173     int iatom,
00174         jatom,
00175         isimp,
00176         jsimp,
00177         gotSimp;
00178     /* Atomic information */
00179     Vatom *atom;
00180     double *position;
00181     /* Simplex/Vertex information */
00182     SS *simplex;
00183     /* Basis function values */
00184
00185     if (thee == VNULL) {
00186         Vnm_print(2, "Vcsn_init: Error! Got NULL thee!\n");
00187         VASSERT(0);
00188     }
00189     if (thee->gm == VNULL) {
00190         Vnm_print(2, "Vcsn_init: Error! Got NULL thee->gm!\n");
00191         VASSERT(0);
00192     }
00193     thee->nsimp = Gem_numSS(thee->gm);
00194     if (thee->nsimp <= 0) {
00195         Vnm_print(2, "Vcsn_init: Error! Got %d simplices!\n", thee->nsimp);
00196         VASSERT(0);
00197     }
00198     thee->natom = Valist_getNumberAtoms(thee->alist);
00199
00200     /* Allocate and initialize space for the first dimensions of the
00201      * simplex-charge map, the simplex array, and the counters */
00202     thee->sqm = (int**)Vmem_malloc(thee->vmem, thee->nsimp, sizeof(int *));
00203     VASSERT(thee->sqm != VNULL);
00204     thee->nsqm = (int*)Vmem_malloc(thee->vmem, thee->nsimp, sizeof(int));

```

```

00205     VASSERT(thee->nsqm != VNULL);
00206     for (isimp=0; isimp<thee->nsimp; isimp++) (thee->nsqm)[isimp] = 0;
00207
00208     /* Count the number of charges per simplex. */
00209     for (iatom=0; iatom<thee->natom; iatom++) {
00210         atom = Valist_getAtom(thee->alist, iatom);
00211         position = Vatom_getPosition(atom);
00212         gotSimp = 0;
00213         for (isimp=0; isimp<thee->nsimp; isimp++) {
00214             simplex = Gem_SS(thee->gm, isimp);
00215             if (Gem_pointInSimplex(thee->gm, simplex, position)) {
00216                 (thee->nsqm)[isimp]++;
00217                 gotSimp = 1;
00218             }
00219         }
00220     }
00221
00222     /* @todo Combine the following two loops? - PCE */
00223     /* Allocate the space for the simplex-charge map */
00224     for (isimp=0; isimp<thee->nsimp; isimp++) {
00225         if ((thee->nsqm)[isimp] > 0) {
00226             thee->sqm[isimp] = (int*)Vmem_malloc(thee->vmem, (thee->nsqm)[isimp],
00227                 sizeof(int));
00228             VASSERT(thee->sqm[isimp] != VNULL);
00229         }
00230     }
00231
00232     /* Finally, set up the map */
00233     for (isimp=0; isimp<thee->nsimp; isimp++) {
00234         jsimp = 0;
00235         simplex = Gem_SS(thee->gm, isimp);
00236         for (iatom=0; iatom<thee->natom; iatom++) {
00237             atom = Valist_getAtom(thee->alist, iatom);
00238             position = Vatom_getPosition(atom);
00239             /* Check to see if the atom's in this simplex */
00240             if (Gem_pointInSimplex(thee->gm, simplex, position)) {
00241                 /* Assign the entries in the next vacant spot */
00242                 (thee->sqm)[isimp][jsimp] = iatom;
00243                 jsimp++;
00244             }
00245         }
00246     }
00247
00248     thee->msimp = thee->nsimp;
00249
00250     /* Allocate space for the charge-simplex map */
00251     thee->qsm = (int**)Vmem_malloc(thee->vmem, thee->natom, sizeof(int *));
00252     VASSERT(thee->qsm != VNULL);
00253     thee->nqsm = (int*)Vmem_malloc(thee->vmem, thee->natom, sizeof(int));
00254     VASSERT(thee->nqsm != VNULL);
00255     for (iatom=0; iatom<thee->natom; iatom++) (thee->nqsm)[iatom] = 0;
00256     /* Loop through the list of simplices and count the number of times
00257        * each atom appears */
00258     for (isimp=0; isimp<thee->nsimp; isimp++) {
00259         for (iatom=0; iatom<thee->nsqm[isimp]; iatom++) {
00260             jatom = thee->sqm[isimp][iatom];
00261             thee->nqsm[jatom]++;
00262         }
00263     }
00264     /* Do a TIME-CONSUMING SANITY CHECK to make sure that each atom was
00265        * placed in at simplex */
00266     for (iatom=0; iatom<thee->natom; iatom++) {
00267         if (thee->nqsm[iatom] == 0) {
00268             Vnm_print(2, "Vcsm_init: Atom %d not placed in simplex!\n", iatom);
00269             VASSERT(0);
00270         }
00271     }
00272     /* Allocate the appropriate amount of space for each entry in the
00273        * charge-simplex map and clear the counter for re-use in assignment */
00274     for (iatom=0; iatom<thee->natom; iatom++) {
00275         thee->qsm[iatom] = (int*)Vmem_malloc(thee->vmem, (thee->nqsm)[iatom],
00276             sizeof(int));
00277         VASSERT(thee->qsm[iatom] != VNULL);
00278         thee->nqsm[iatom] = 0;
00279     }
00280     /* Assign the simplices to atoms */
00281     for (isimp=0; isimp<thee->nsimp; isimp++) {
00282         for (iatom=0; iatom<thee->nsqm[isimp]; iatom++) {
00283             jatom = thee->sqm[isimp][iatom];
00284             thee->qsm[jatom][thee->nqsm[jatom]] = isimp;
00285             thee->nqsm[jatom]++;

```

```

00286     }
00287 }
00288
00289     thee->initFlag = 1;
00290 }
00291
00292 VPUBLIC void Vcsbm_dtor(Vcsbm **thee) {
00293     if ((*thee) != VNULL) {
00294         Vcsbm_dtor2(*thee);
00295         Vmem_free(VNULL, 1, sizeof(Vcsbm), (void **)thee);
00296         (*thee) = VNULL;
00297     }
00298 }
00299
00300 VPUBLIC void Vcsbm_dtor2(Vcsbm *thee) {
00301     int i;
00302
00303     if ((thee != VNULL) && thee->initFlag) {
00304
00305         for (i=0; i<thee->msimp; i++) {
00306             if (thee->nsqm[i] > 0) Vmem_free(thee->vmem, thee->nsqm[i],
00307                 sizeof(int), (void *)&(thee->sqm[i]));
00308         }
00309         for (i=0; i<thee->natom; i++) {
00310             if (thee->nqsm[i] > 0) Vmem_free(thee->vmem, thee->nqsm[i],
00311                 sizeof(int), (void *)&(thee->qsm[i]));
00312         }
00313         Vmem_free(thee->vmem, thee->msimp, sizeof(int *),
00314             (void *)&(thee->sqm));
00315         Vmem_free(thee->vmem, thee->msimp, sizeof(int),
00316             (void *)&(thee->nsqm));
00317         Vmem_free(thee->vmem, thee->natom, sizeof(int *),
00318             (void *)&(thee->qsm));
00319         Vmem_free(thee->vmem, thee->natom, sizeof(int),
00320             (void *)&(thee->nqsm));
00321     }
00322 }
00323 Vmem_dtor(&(thee->vmem));
00324 }
00325
00326 VPUBLIC int Vcsbm_update(Vcsbm *thee, SS **simps, int num) {
00327
00328     /* Counters */
00329     int isimp, jsimp, iatom, jatom, atomID, simpID;
00330     int nsimps, gotMem;
00331     /* Object info */
00332     Vatom *atom;
00333     SS *simplex;
00334     double *position;
00335     /* Lists */
00336     int *qParent, nqParent;
00337     int **sqmNew, *nsqmNew;
00338     int *affAtoms, nAffAtoms;
00339     int *dnqsm, *nqsmNew, **qsmNew;
00340
00341     VASSERT(thee != VNULL);
00342     VASSERT(thee->initFlag);
00343
00344     /* If we don't have enough memory to accommodate the new entries,
00345      * add more by doubling the existing amount */
00346     isimp = thee->nsimp + num - 1;
00347     gotMem = 0;
00348     while (!gotMem) {
00349         if (isimp > thee->msimp) {
00350             isimp = 2 * isimp;
00351             thee->nsqm = (int*)Vmem_realloc(thee->vmem, thee->msimp, sizeof(int),
00352                 (void *)&(thee->nsqm), isimp);
00353             VASSERT(thee->nsqm != VNULL);
00354             thee->sqm = (int**)Vmem_realloc(thee->vmem, thee->msimp, sizeof(int *),
00355                 (void *)&(thee->sqm), isimp);
00356             VASSERT(thee->sqm != VNULL);
00357             thee->msimp = isimp;
00358         } else gotMem = 1;
00359     }
00360     /* Initialize the nsqm entires we just allocated */
00361     for (isimp = thee->nsimp; isimp<thee->nsimp+num-1; isimp++) {
00362         thee->nsqm[isimp] = 0;
00363     }
00364
00365     thee->nsimp = thee->nsimp + num - 1;
00366

```

```

00367     /* There's a simple case to deal with: if simps[0] didn't have a
00368     * charge in the first place */
00369     isimp = SS_id(simps[0]);
00370     if (thee->nsqm[isimp] == 0) {
00371         for (isimp=1; isimp<num; isimp++) {
00372             thee->nsqm[SS_id(simps[isimp])] = 0;
00373         }
00374         return 1;
00375     }
00376
00377     /* The more complicated case has occurred; the parent simplex had one or
00378     * more charges. First, generate the list of affected charges. */
00379     isimp = SS_id(simps[0]);
00380     nqParent = thee->nsqm[isimp];
00381     qParent = thee->sqm[isimp];
00382
00383     sqmNew = (int**)Vmem_malloc(thee->vmem, num, sizeof(int *));
00384     VASSERT(sqmNew != VNULL);
00385     nsqmNew = (int*)Vmem_malloc(thee->vmem, num, sizeof(int));
00386     VASSERT(nsqmNew != VNULL);
00387     for (isimp=0; isimp<num; isimp++) nsqmNew[isimp] = 0;
00388
00389     /* Loop through the affected atoms to determine how many atoms each
00390     * simplex will get. */
00391     for (iatom=0; iatom<nqParent; iatom++) {
00392
00393         atomID = qParent[iatom];
00394         atom = Valist_getAtom(thee->alist, atomID);
00395         position = Vatom_getPosition(atom);
00396         nsimps = 0;
00397
00398         jsimp = 0;
00399
00400         for (isimp=0; isimp<num; isimp++) {
00401             simplex = simps[isimp];
00402             if (Gem_pointInSimplex(thee->gm, simplex, position)) {
00403                 nsqmNew[isimp]++;
00404                 jsimp = 1;
00405             }
00406         }
00407
00408         VASSERT(jsimp != 0);
00409     }
00410
00411     /* Sanity check that we didn't lose any atoms... */
00412     iatom = 0;
00413     for (isimp=0; isimp<num; isimp++) iatom += nsqmNew[isimp];
00414     if (iatom < nqParent) {
00415         Vnm_print(2, "Vcsm_update: Lost %d (of %d) atoms!\n",
00416                 nqParent - iatom, nqParent);
00417         VASSERT(0);
00418     }
00419
00420     /* Allocate the storage */
00421     for (isimp=0; isimp<num; isimp++) {
00422         if (nsqmNew[isimp] > 0) {
00423             sqmNew[isimp] = (int*)Vmem_malloc(thee->vmem, nsqmNew[isimp],
00424                 sizeof(int));
00425             VASSERT(sqmNew[isimp] != VNULL);
00426         }
00427     }
00428
00429     /* Assign charges to simplices */
00430     for (isimp=0; isimp<num; isimp++) {
00431
00432         jsimp = 0;
00433         simplex = simps[isimp];
00434
00435         /* Loop over the atoms associated with the parent simplex */
00436         for (iatom=0; iatom<nqParent; iatom++) {
00437
00438             atomID = qParent[iatom];
00439             atom = Valist_getAtom(thee->alist, atomID);
00440             position = Vatom_getPosition(atom);
00441             if (Gem_pointInSimplex(thee->gm, simplex, position)) {
00442                 sqmNew[isimp][jsimp] = atomID;
00443                 jsimp++;
00444             }
00445         }
00446     }
00447

```

```

00448      /* Update the QSM map using the old and new SQM lists */
00449      /* The affected atoms are those contained in the parent simplex; i.e.
00450       * thee->sqm[SS_id(simps[0])] */
00451      affAtoms = thee->sqm[SS_id(simps[0])];
00452      nAffAtoms = thee->nsqm[SS_id(simps[0])];
00453      /* Each of these atoms will go somewhere else; i.e., the entries in
00454       * thee->qsm are never destroyed and thee->nqsm never decreases.
00455       * However, it is possible that a subdivision could cause an atom to be
00456       * shared by two child simplices. Here we record the change, if any,
00457       * in the number of simplices associated with each atom. */
00458      dnqsm = (int*)Vmem_malloc(thee->vmem, nAffAtoms, sizeof(int));
00459      VASSERT(dnqsm != VNULL);
00460      nqsmNew = (int*)Vmem_malloc(thee->vmem, nAffAtoms, sizeof(int));
00461      VASSERT(nqsmNew != VNULL);
00462      qsmNew = (int**)Vmem_malloc(thee->vmem, nAffAtoms, sizeof(int*));
00463      VASSERT(qsmNew != VNULL);
00464      for (iatom=0; iatom<nAffAtoms; iatom++) {
00465          dnqsm[iatom] = -1;
00466          atomID = affAtoms[iatom];
00467          for (isimp=0; isimp<num; isimp++) {
00468              for (jatom=0; jatom<nqsmNew[isimp]; jatom++) {
00469                  if (qsmNew[isimp][jatom] == atomID) dnqsm[iatom]++;
00470              }
00471          }
00472          VASSERT(dnqsm[iatom] > -1);
00473      }
00474      /* Setup the new entries in the array */
00475      for (iatom=0; iatom<nAffAtoms; iatom++) {
00476          atomID = affAtoms[iatom];
00477          qsmNew[iatom] = (int*)Vmem_malloc(thee->vmem,
00478              (dnqsm[iatom] + thee->nqsm[atomID]),
00479              sizeof(int));
00480          nqsmNew[iatom] = 0;
00481          VASSERT(qsmNew[iatom] != VNULL);
00482      }
00483      /* Fill the new entries in the array */
00484      /* First, do the modified entries */
00485      for (isimp=0; isimp<num; isimp++) {
00486          simpID = SS_id(simps[isimp]);
00487          for (iatom=0; iatom<nqsmNew[isimp]; iatom++) {
00488              atomID = qsmNew[isimp][iatom];
00489              for (jatom=0; jatom<nAffAtoms; jatom++) {
00490                  if (atomID == affAtoms[jatom]) break;
00491              }
00492              if (jatom < nAffAtoms) {
00493                  qsmNew[jatom][nqsmNew[jatom]] = simpID;
00494                  nqsmNew[jatom]++;
00495              }
00496          }
00497      }
00498      /* Now do the unmodified entries */
00499      for (iatom=0; iatom<nAffAtoms; iatom++) {
00500          atomID = affAtoms[iatom];
00501          for (isimp=0; isimp<thee->nqsm[atomID]; isimp++) {
00502              for (jsimp=0; jsimp<num; jsimp++) {
00503                  simpID = SS_id(simps[jsimp]);
00504                  if (thee->qsm[atomID][isimp] == simpID) break;
00505              }
00506              if (jsimp == num) {
00507                  qsmNew[iatom][nqsmNew[iatom]] = thee->qsm[atomID][isimp];
00508                  nqsmNew[iatom]++;
00509              }
00510          }
00511      }
00512
00513      /* Replace the existing entries in the table. Do the QSM entires
00514       * first, since they require affAtoms = thee->sqm[simps[0]] */
00515      for (iatom=0; iatom<nAffAtoms; iatom++) {
00516          atomID = affAtoms[iatom];
00517          Vmem_free(thee->vmem, thee->nqsm[atomID], sizeof(int),
00518              (void **)&(thee->qsm[atomID]));
00519          thee->qsm[atomID] = qsmNew[iatom];
00520          thee->nqsm[atomID] = nqsmNew[iatom];
00521      }
00522      for (isimp=0; isimp<num; isimp++) {
00523          simpID = SS_id(simps[isimp]);
00524          if (thee->nsqm[simpID] > 0) Vmem_free(thee->vmem, thee->nsqm[simpID],
00525              sizeof(int), (void **)&(thee->sqm[simpID]));
00526          thee->sqm[simpID] = qsmNew[isimp];
00527          thee->nqsm[simpID] = nqsmNew[isimp];
00528      }

```

```

00529
00530     Vmem_free(thee->vmem, num, sizeof(int *), (void **)&sqmNew);
00531     Vmem_free(thee->vmem, num, sizeof(int), (void **)&nsgmNew);
00532     Vmem_free(thee->vmem, nAffAtoms, sizeof(int *), (void **)&qsmNew);
00533     Vmem_free(thee->vmem, nAffAtoms, sizeof(int), (void **)&nqsmNew);
00534     Vmem_free(thee->vmem, nAffAtoms, sizeof(int), (void **)&dnqsm);
00535
00536
00537     return 1;
00538
00539
00540 }

```

9.6 src/fem/vcsm.h File Reference

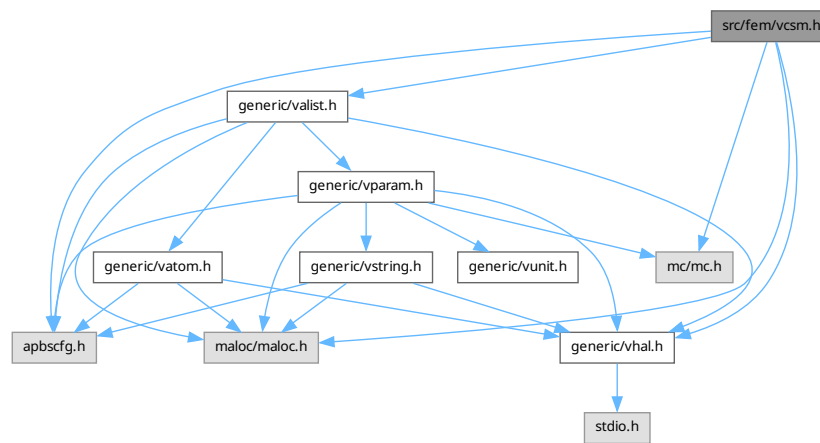
Contains declarations for the Vcsm class.

```

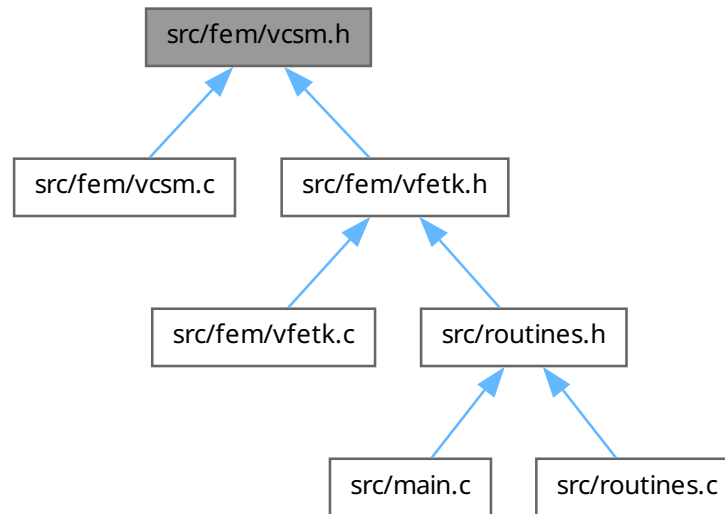
#include "apbscfg.h"
#include "maloc/maloc.h"
#include "mc/mc.h"
#include "generic/vhal.h"
#include "generic/valist.h"

```

Include dependency graph for vcsm.h:



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [sVcsm](#)
Charge-simplex map class.

Typedefs

- typedef struct [sVcsm](#) [Vcsm](#)
Declaration of the Vcsm class as the Vcsm structure.

Functions

- VEXTERNC void [Gem_setExternalUpdateFunction](#) ([Gem](#) *thee, void(*externalUpdate)(SS **simps, int num))
External function for FEtk Gem class to use during mesh refinement.
- VEXTERNC [Valist](#) * [Vcsm_getValist](#) ([Vcsm](#) *thee)
Get atom list.
- VEXTERNC int [Vcsm_getNumberAtoms](#) ([Vcsm](#) *thee, int isimp)
Get number of atoms associated with a simplex.
- VEXTERNC [Vatom](#) * [Vcsm_getAtom](#) ([Vcsm](#) *thee, int iatom, int isimp)
Get particular atom associated with a simplex.
- VEXTERNC int [Vcsm_getAtomIndex](#) ([Vcsm](#) *thee, int iatom, int isimp)
Get ID of particular atom in a simplex.
- VEXTERNC int [Vcsm_getNumberSimplexes](#) ([Vcsm](#) *thee, int iatom)
Get number of simplexes associated with an atom.
- VEXTERNC SS * [Vcsm_getSimplex](#) ([Vcsm](#) *thee, int isimp, int iatom)
Get particular simplex associated with an atom.

- VEXTERNC int [Vcsm_getSimplexIndex](#) ([Vcsm](#) *thee, int isimp, int iatom)
Get index particular simplex associated with an atom.
- VEXTERNC unsigned long int [Vcsm_memChk](#) ([Vcsm](#) *thee)
Return the memory used by this structure (and its contents) in bytes.
- VEXTERNC [Vcsm](#) * [Vcsm_ctor](#) ([Valist](#) *alist, [Gem](#) *gm)
Construct Vcsm object.
- VEXTERNC int [Vcsm_ctor2](#) ([Vcsm](#) *thee, [Valist](#) *alist, [Gem](#) *gm)
FORTTRAN stub to construct Vcsm object.
- VEXTERNC void [Vcsm_dtor](#) ([Vcsm](#) **thee)
Destroy Vcsm object.
- VEXTERNC void [Vcsm_dtor2](#) ([Vcsm](#) *thee)
FORTTRAN stub to destroy Vcsm object.
- VEXTERNC void [Vcsm_init](#) ([Vcsm](#) *thee)
Initialize charge-simplex map with mesh and atom data.
- VEXTERNC int [Vcsm_update](#) ([Vcsm](#) *thee, [SS](#) **simps, int num)
Update the charge-simplex and simplex-charge maps after refinement.

9.6.1 Detailed Description

Contains declarations for the Vcsm class.

Version

\$Id\$

Author

Nathan A. Baker

Attention

```
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*
*

```

Definition in file [vcsbm.h](#).

9.7 vcsbm.h

[Go to the documentation of this file.](#)

```

00001
00063 #ifndef _VCSM_H_
00064 #define _VCSM_H_
00065
00066 #include "apbscfg.h"
00067
00068 #include "malloc/malloc.h"
00069 #include "mc/mc.h"
00070
00071 #include "generic/vhal.h"
00072 #include "generic/valist.h"
00073
00078 VEXTERN void Gem_setExternalUpdateFunction(
00079     Gem *thee,
00080     void (*externalUpdate)(SS **sims, int num)
00083 );
00084
00089 struct sVcsm {
00090
00091     Valist *alist;
00092     int natom;
00094     Gem *gm;
00097     int **sqm;
00104     int *nsqm;
00105     int nsimp;
00107     int msimp;
00109     int **qsm;
00111     int *nqsm;
00112     int initFlag;
00114     Vmem *vmem;
00116 };
00117
00122 typedef struct sVcsm Vcsm;
00123
00124 /* ////////////////////////////////////////
00125 // Class Vcsm: Inlineable methods (vcsbm.c)
00127
00128 #if !defined(VINLINE_VCSM)
00129
00135     VEXTERN Valist* Vcsm_getValist(
00136         Vcsm *thee /**< The Vcsm object */
00137     );
00138
00144     VEXTERN int Vcsm_getNumberAtoms(
00145         Vcsm *thee,
00146         int isimp
00147     );
00148
00154     VEXTERN Vatom* Vcsm_getAtom(
00155         Vcsm *thee,

```

```

00156         int iatom,
00157         int isimp
00158     );
00159
00165     VEXTERNC int Vcsm_getAtomIndex(
00166         Vcsm *thee,
00167         int iatom,
00168         int isimp
00169     );
00170
00176     VEXTERNC int Vcsm_getNumberSimplices(
00177         Vcsm *thee,
00178         int iatom
00179     );
00180
00186     VEXTERNC SS* Vcsm_getSimplex(
00187         Vcsm *thee,
00188         int isimp,
00189         int iatom
00190     );
00191
00197     VEXTERNC int Vcsm_getSimplexIndex(
00198         Vcsm *thee,
00199         int isimp,
00200         int iatom
00201     );
00202
00209     VEXTERNC unsigned long int Vcsm_memChk(
00210         Vcsm *thee
00211     );
00212
00213 #else /* if defined(VINLINE_VCSM) */
00214 #   define Vcsm_getValist(thee) ((thee)->alist)
00215 #   define Vcsm_getNumberAtoms(thee, isimp) ((thee)->nsgm[isimp])
00216 #   define Vcsm_getAtom(thee, iatom, isimp) (Valist_getAtom((thee)->alist, ((thee)->sgm)[isimp][iatom]))
00217 #   define Vcsm_getAtomIndex(thee, iatom, isimp) (((thee)->sgm)[isimp][iatom])
00218 #   define Vcsm_getNumberSimplices(thee, iatom) (((thee)->nqsm)[iatom])
00219 #   define Vcsm_getSimplex(thee, isimp, iatom) (Gem_SS((thee)->gm, ((thee)->qsm)[iatom][isimp]))
00220 #   define Vcsm_getSimplexIndex(thee, isimp, iatom) (((thee)->qsm)[iatom][isimp])
00221 #   define Vcsm_memChk(thee) (Vmem_bytes((thee)->vmem))
00222 #endif /* if !defined(VINLINE_VCSM) */
00223
00224 /* ////////////////////////////////////// */
00225 // Class Vcsm: Non-Inlineable methods (vcsm.c)
00226
00236 VEXTERNC Vcsm* Vcsm_ctor(
00237     Valist *alist, /**< List of atoms */
00238     Gem *gm
00239 );
00240
00249 VEXTERNC int Vcsm_ctor2(
00250     Vcsm *thee,
00251     Valist *alist,
00252     Gem *gm
00253 );
00254
00259 VEXTERNC void Vcsm_dtor(
00260     Vcsm **thee
00261 );
00262
00267 VEXTERNC void Vcsm_dtor2(
00268     Vcsm *thee
00269 );
00270
00277 VEXTERNC void Vcsm_init(
00278     Vcsm *thee
00279 );
00280
00287 VEXTERNC int Vcsm_update(
00288     Vcsm *thee,
00289     SS **simps,
00294     int num
00295 );
00296
00297 #endif /* ifndef _VCSM_H_ */

```


- Return the total electrostatic energy.*
- VPUBLIC double [Vfetk_qfEnergy](#) ([Vfetk](#) *thee, int color)
- Get the "fixed charge" contribution to the electrostatic energy.*
- VPUBLIC double [Vfetk_dqmEnergy](#) ([Vfetk](#) *thee, int color)
- Get the "mobile charge" and "polarization" contributions to the electrostatic energy.*
- VPUBLIC void [Vfetk_setAtomColors](#) ([Vfetk](#) *thee)
- Transfer color (partition ID) information frmo a partitioned mesh to the atoms.*
- VPUBLIC unsigned long int [Vfetk_memChk](#) ([Vfetk](#) *thee)
- Return the memory used by this structure (and its contents) in bytes.*
- VPUBLIC Vrc_Codes [Vfetk_genCube](#) ([Vfetk](#) *thee, double center[3], double length[3], [Vfetk_MeshLoad](#) mesh←Type)
- Construct a rectangular mesh (in the current Vfetk object)*
- VPUBLIC Vrc_Codes [Vfetk_loadMesh](#) ([Vfetk](#) *thee, double center[3], double length[3], [Vfetk_MeshLoad](#) mesh←Type, Vio *sock)
- Loads a mesh into the Vfetk (and associated) object(s).*
- VPUBLIC void [Bmat_printHB](#) (Bmat *thee, char *fname)
- Writes a Bmat to disk in Harwell-Boeing sparse matrix format.*
- VPUBLIC PDE * [Vfetk_PDE_ctor](#) ([Vfetk](#) *fetk)
- Constructs the FEtk PDE object.*
- VPUBLIC int [Vfetk_PDE_ctor2](#) (PDE *thee, [Vfetk](#) *fetk)
- Intializes the FEtk PDE object.*
- VPUBLIC void [Vfetk_PDE_dtor](#) (PDE **thee)
- Destroys FEtk PDE object.*
- VPUBLIC void [Vfetk_PDE_dtor2](#) (PDE *thee)
- FORTTRAN stub: destroys FEtk PDE object.*
- VPUBLIC void [Vfetk_PDE_initAssemble](#) (PDE *thee, int ip[], double rp[])
- Do once-per-assembly initialization.*
- VPUBLIC void [Vfetk_PDE_initElement](#) (PDE *thee, int elementType, int chart, double txq[][3], void *data)
- VPUBLIC void [Vfetk_PDE_initFace](#) (PDE *thee, int faceType, int chart, double tnvect[])
- Do once-per-face initialization.*
- VPUBLIC void [Vfetk_PDE_initPoint](#) (PDE *thee, int pointType, int chart, double txq[], double tU[], double tdU[][3])
- VPUBLIC void [Vfetk_PDE_Fu](#) (PDE *thee, int key, double F[])
- Evaluate strong form of PBE. For interior points, this is:*
- VPUBLIC double [Vfetk_PDE_Fu_v](#) (PDE *thee, int key, double V[], double dV[][[VAPBS_DIM](#)])
- This is the weak form of the PBE; i.e. the strong form integrated with a test function to give:*
- VPUBLIC double [Vfetk_PDE_DF_u_vv](#) (PDE *thee, int key, double W[], double dW[][[VAPBS_DIM](#)], double V[], double dV[][3])
- VPUBLIC void [Vfetk_PDE_delta](#) (PDE *thee, int type, int chart, double txq[], void *user, double F[])
- Evaluate a (discretized) delta function source term at the given point.*
- VPUBLIC void [Vfetk_PDE_u_D](#) (PDE *thee, int type, int chart, double txq[], double F[])
- Evaluate the Dirichlet boundary condition at the given point.*
- VPUBLIC void [Vfetk_PDE_u_T](#) (PDE *thee, int type, int chart, double txq[], double F[])
- Evaluate the "true solution" at the given point for comparison with the numerical solution.*
- VPUBLIC void [Vfetk_PDE_bisectEdge](#) (int dim, int dimII, int edgeType, int chart[], double vx[][3])
- VPUBLIC void [Vfetk_PDE_mapBoundary](#) (int dim, int dimII, int vertexType, int chart, double vx[3])
- VPUBLIC int [Vfetk_PDE_markSimplex](#) (int dim, int dimII, int simplexType, int faceType[[VAPBS_NVS](#)], int vertex←Type[[VAPBS_NVS](#)], int chart[], double vx[][3], void *simplex)
- VPUBLIC void [Vfetk_PDE_oneChart](#) (int dim, int dimII, int objType, int chart[], double vx[][3], int dimV)

- VPUBLIC double [Vfetk_PDE_Ju](#) (PDE *thee, int key)
Energy functional. This returns the energy (less delta function terms) in the form:
- VPUBLIC void [Vfetk_externalUpdateFunction](#) (SS **simps, int num)
External hook to simplex subdivision routines in Gem. Called each time a simplex is subdivided (we use it to update the charge-simplex map)
- VPUBLIC int [Vfetk_PDE_simplexBasisInit](#) (int key, int dim, int comp, int *ndof, int dof[])
Initialize the bases for the trial or the test space, for a particular component of the system, at all quadrature points on the master simplex element.
- VPUBLIC void [Vfetk_PDE_simplexBasisForm](#) (int key, int dim, int comp, int pdkey, double xq[], double basis[])
Evaluate the bases for the trial or test space, for a particular component of the system, at all quadrature points on the master simplex element.
- VPUBLIC void [Vfetk_dumpLocalVar](#) ()
Debugging routine to print out local variables used by PDE object.
- VPUBLIC int [Vfetk_fillArray](#) (Vfetk *thee, Bvec *vec, Vdata_Type type)
Fill an array with the specified data.
- VPUBLIC int [Vfetk_write](#) (Vfetk *thee, const char *iodev, const char *iofmt, const char *thost, const char *fname, Bvec *vec, Vdata_Format format)
Write out data.

Variables

- VPRIVATE [Vfetk_LocalVar](#) var
- VPRIVATE char * [diriCubeString](#)
- VPRIVATE char * [neumCubeString](#)
- VPRIVATE int [dim_2DP1](#) = 3
- VPRIVATE int [lgr_2DP1](#) [3][VMAXP]
- VPRIVATE int [lgr_2DP1x](#) [3][VMAXP]
- VPRIVATE int [lgr_2DP1y](#) [3][VMAXP]
- VPRIVATE int [lgr_2DP1z](#) [3][VMAXP]
- VPRIVATE int [dim_3DP1](#) = [VAPBS_NVS](#)
- VPRIVATE int [lgr_3DP1](#) [[VAPBS_NVS](#)][VMAXP]
- VPRIVATE int [lgr_3DP1x](#) [[VAPBS_NVS](#)][VMAXP]
- VPRIVATE int [lgr_3DP1y](#) [[VAPBS_NVS](#)][VMAXP]
- VPRIVATE int [lgr_3DP1z](#) [[VAPBS_NVS](#)][VMAXP]
- VPRIVATE const int [P_DEG](#) =1
- VPRIVATE int [numP](#)
- VPRIVATE double [c](#) [VMAXP][VMAXP]
- VPRIVATE double [cx](#) [VMAXP][VMAXP]
- VPRIVATE double [cy](#) [VMAXP][VMAXP]
- VPRIVATE double [cz](#) [VMAXP][VMAXP]

9.8.1 Detailed Description

Class Vfetk methods.

Author

Nathan Baker

Version

\$Id\$

Attention

```

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*
*

```

Definition in file [vfetk.c](#).

9.8.2 Function Documentation**9.8.2.1 polyEval()**

```

VPRIVATE void polyEval (
    int numP,
    double p[],
    double c[][VMAXP],
    double xv[] )

```

Definition at line [2095](#) of file [vfetk.c](#).

9.8.2.2 Vfetk_PDE_bisectEdge()

```

VPUBLIC void Vfetk_PDE_bisectEdge (

```

```

    int dim,
    int dimII,
    int edgeType,
    int chart[],
    double vx[][3] )

```

Definition at line 1902 of file [vfetc.c](#).

9.8.2.3 Vfetc_PDE_DFu_wv()

```

VPUBLIC double Vfetc_PDE_DFu_wv (
    PDE * thee,
    int key,
    double W[],
    double dW[][VAPBS_DIM],
    double V[],
    double dV[][3] )

```

Definition at line 1741 of file [vfetc.c](#).

9.8.2.4 Vfetc_PDE_initElement()

```

VPUBLIC void Vfetc_PDE_initElement (
    PDE * thee,
    int elementType,
    int chart,
    double tvx[][3],
    void * data )

```

Definition at line 1528 of file [vfetc.c](#).

9.8.2.5 Vfetc_PDE_initPoint()

```

VPUBLIC void Vfetc_PDE_initPoint (
    PDE * thee,
    int pointType,
    int chart,
    double txq[],
    double tU[],
    double tdU[][3] )

```

Definition at line 1571 of file [vfetc.c](#).

9.8.2.6 Vfetc_PDE_mapBoundary()

```

VPUBLIC void Vfetc_PDE_mapBoundary (
    int dim,
    int dimII,
    int vertexType,
    int chart,
    double vx[3] )

```

Definition at line 1912 of file [vfetc.c](#).

9.8.2.7 Vfetc_PDE_markSimplex()

```

VPUBLIC int Vfetc_PDE_markSimplex (
    int dim,
    int dimII,
    int simplexType,

```

```

    int faceType[VAPBS_NVS],
    int vertexType[VAPBS_NVS],
    int chart[],
    double vx[][3],
    void * simplex )

```

Definition at line 1917 of file [vfetk.c](#).

9.8.2.8 Vfetk_PDE_oneChart()

```

VPUBLIC void Vfetk_PDE_oneChart (
    int dim,
    int dimII,
    int objType,
    int chart[],
    double vx[][3],
    int dimV )

```

Definition at line 1998 of file [vfetk.c](#).

9.8.3 Variable Documentation

9.8.3.1 c

```
VPRIVATE double c[VMAXP][VMAXP]
```

Definition at line 483 of file [vfetk.c](#).

9.8.3.2 cx

```
VPRIVATE double cx[VMAXP][VMAXP]
```

Definition at line 484 of file [vfetk.c](#).

9.8.3.3 cy

```
VPRIVATE double cy[VMAXP][VMAXP]
```

Definition at line 485 of file [vfetk.c](#).

9.8.3.4 cz

```
VPRIVATE double cz[VMAXP][VMAXP]
```

Definition at line 486 of file [vfetk.c](#).

9.8.3.5 dim_2DP1

```
VPRIVATE int dim_2DP1 = 3
```

Definition at line 366 of file [vfetk.c](#).

9.8.3.6 dim_3DP1

```
VPRIVATE int dim_3DP1 = VAPBS_NVS
```

Definition at line 437 of file [vfetk.c](#).

9.8.3.7 diriCubeString

```
VPRIVATE char* diriCubeString
```

Definition at line 93 of file [vfetk.c](#).

9.8.3.8 lgr_2DP1

```
VPRIVATE int lgr_2DP1[3][VMAXP]
```

Initial value:

```
= {
```

```
{ 2, -2, -2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
{ 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
{ 0, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 }
}
```

Definition at line 386 of file [vfetk.c](#).

9.8.3.9 lgr_2DP1x

```
VPRIVATE int lgr_2DP1x[3][VMAXP]
```

Initial value:

```
= {
```

```
{ -2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
{ 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
{ 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 }
}
```

Definition at line 395 of file [vfetk.c](#).

9.8.3.10 lgr_2DP1y

```
VPRIVATE int lgr_2DP1y[3][VMAXP]
```

Initial value:

```
= {
```

```
{ -2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
{ 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
{ 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 }
}
```

Definition at line 402 of file [vfetk.c](#).

9.8.3.11 lgr_2DP1z

```
VPRIVATE int lgr_2DP1z[3][VMAXP]
```

Initial value:

```
= {
```

```
{ 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
{ 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
{ 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 }
}
```

Definition at line 409 of file [vfetk.c](#).

9.8.3.12 lgr_3DP1

```
VPRIVATE int lgr_3DP1[VAPBS_NVS][VMAXP]
```

Initial value:

```
= {
```

```
{ 2, -2, -2, -2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
{ 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
{ 0, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
{ 0, 0, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 }
}
```

Definition at line 438 of file [vfetk.c](#).

9.8.3.13 lgr_3DP1x

```
VPRIVATE int lgr_3DP1x[VAPBS_NVS][VMAXP]
```

Initial value:

```
= {
```

```
{ -2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
{ 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
{ 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
{ 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 }
}
```

Definition at line 446 of file [vfetk.c](#).

9.8.3.14 lgr_3DP1y

```
VPRIVATE int lgr_3DP1y[VAPBS_NVS][VMAXP]
```

Initial value:

```
= {
```

```
{ -2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
{ 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
{ 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
{ 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 }
}
```

Definition at line 454 of file [vfetk.c](#).

9.8.3.15 lgr_3DP1z

```
VPRIVATE int lgr_3DP1z[VAPBS_NVS][VMAXP]
```

Initial value:

```
= {
```

```
{ -2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
{ 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
{ 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
{ 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 }
}
```

Definition at line 462 of file [vfetk.c](#).

9.8.3.16 neumCubeString

```
VPRIVATE char* neumCubeString
```

Definition at line 130 of file [vfetk.c](#).

9.8.3.17 numP

```
VPRIVATE int numP
```

Definition at line 482 of file [vfetk.c](#).

9.8.3.18 P_DEG

```
VPRIVATE const int P_DEG =1
```

Definition at line 476 of file [vfetk.c](#).

9.8.3.19 var

```
VPRIVATE Vfetk_LocalVar var
```

Definition at line 86 of file [vfetk.c](#).

9.9 vfetk.c

[Go to the documentation of this file.](#)

```

00001
00057 #include "vfetk.h"
00058
00059 /* Define the macro DONEUMANN to run with all-Neumann boundary conditions.
00060  * Set this macro at your own risk! */
00061 /* #define DONEUMANN 1 */
00062
00063 /*
00064  * @brief Calculate the contribution to the charge-potential energy from one
00065  * atom
00066  * @ingroup Vfetk
00067  * @author Nathan Baker
00068  * @param thee current Vfetk object
00069  * @param iatom current atom index
00070  * @param color simplex subset (partition) under consideration
00071  * @param sol current solution
00072  * @returns Per-atom energy
00073  */
00074 VPRIVATE double Vfetk_qfEnergyAtom(
00075     Vfetk *thee,
00076     int iatom,
00077     int color,
00078     double *sol
00079 );
00080
00081 /*
00082  * @brief Container for local variables
00083  * @ingroup Vfetk
00084  * @bug Not thread-safe
00085  */
00086 VPRIVATE Vfetk_LocalVar var;
00087
00088 /*
00089  * @brief MCSF-format cube mesh (all Dirichlet)
00090  * @ingroup Vfetk
00091  * @author Based on mesh by Mike Holst
00092  */
00093 VPRIVATE char *diriCubeString =
00094 "mcsf_begin=1;\n\
00095 \n\
00096 dim=3;\n\
00097 dimii=3;\n\
00098 vertices=8;\n\
00099 simplices=6;\n\
00100 \n\
00101 vert=[\n\
00102 0 0 -0.5 -0.5 -0.5\n\
00103 1 0 0.5 -0.5 -0.5\n\
00104 2 0 -0.5 0.5 -0.5\n\
00105 3 0 0.5 0.5 -0.5\n\
00106 4 0 -0.5 -0.5 0.5\n\
00107 5 0 0.5 -0.5 0.5\n\
00108 6 0 -0.5 0.5 0.5\n\
00109 7 0 0.5 0.5 0.5\n\
00110 ];\n\
00111 \n\
00112 simp=[\n\
00113 0 0 0 0 1 0 1 0 5 1 2\n\
00114 1 0 0 0 1 1 0 0 5 2 4\n\
00115 2 0 0 0 1 0 1 1 5 3 2\n\
00116 3 0 0 0 1 0 1 3 5 7 2\n\
00117 4 0 0 1 1 0 0 2 5 7 6\n\
00118 5 0 0 1 1 0 0 2 5 6 4\n\
00119 ];\n\
00120 \n\
00121 mcsf_end=1;\n\
00122 \n\
00123 ";
00124
00125 /*
00126  * @brief MCSF-format cube mesh (all Neumann)
00127  * @ingroup Vfetk
00128  * @author Based on mesh by Mike Holst
00129  */
00130 VPRIVATE char *neumCubeString =
00131 "mcsf_begin=1;\n\
00132 \n\

```

```

00133 dim=3;\n\
00134 dimii=3;\n\
00135 vertices=8;\n\
00136 simplices=6;\n\
00137 \n\
00138 vert=[\n\
00139 0 0 -0.5 -0.5 -0.5\n\
00140 1 0 0.5 -0.5 -0.5\n\
00141 2 0 -0.5 0.5 -0.5\n\
00142 3 0 0.5 0.5 -0.5\n\
00143 4 0 -0.5 -0.5 0.5\n\
00144 5 0 0.5 -0.5 0.5\n\
00145 6 0 -0.5 0.5 0.5\n\
00146 7 0 0.5 0.5 0.5\n\
00147 ];\n\
00148 \n\
00149 simp=[\n\
00150 0 0 0 0 2 0 2 0 5 1 2\n\
00151 1 0 0 0 2 2 0 0 5 2 4\n\
00152 2 0 0 0 2 0 2 1 5 3 2\n\
00153 3 0 0 0 2 0 2 3 5 7 2\n\
00154 4 0 0 2 2 0 0 2 5 7 6\n\
00155 5 0 0 2 2 0 0 2 5 6 4\n\
00156 ];\n\
00157 \n\
00158 mcsf_end=1;\n\
00159 \n\
00160 ";
00161
00162 /*
00163  * @brief Return the smoothed value of the dielectric coefficient at the
00164  * current point using a fast, chart-based method
00165  * @ingroup Vfetk
00166  * @author Nathan Baker
00167  * @returns Value of dielectric coefficient
00168  * @bug Not thread-safe
00169  */
00170 VPRIVATE double diel();
00171
00172 /*
00173  * @brief Return the smoothed value of the ion accessibility at the
00174  * current point using a fast, chart-based method
00175  * @ingroup Vfetk
00176  * @author Nathan Baker
00177  * @returns Value of mobile ion coefficient
00178  * @bug Not thread-safe
00179  */
00180 VPRIVATE double ionacc();
00181
00182 /*
00183  * @brief Smooths a mesh-based coefficient with a simple harmonic function
00184  * @ingroup Vfetk
00185  * @author Nathan Baker
00186  * @param meth Method for smoothing
00187  * \li 0 ==> arithmetic mean (gives bad results)
00188  * \li 1 ==> geometric mean
00189  * @param nverts Number of vertices
00190  * @param dist distance from point to each vertex
00191  * @param coeff coefficient value at each vertex
00192  * @note Thread-safe
00193  * @return smoothed value of coefficient at point of interest */
00194 VPRIVATE double smooth(
00195     int nverts,
00196     double dist[VAPBS_NVS],
00197     double coeff[VAPBS_NVS],
00198     int meth
00199 );
00200
00201
00202 /*
00203  * @brief Return the analytical multi-sphere Debye-Huckel approximation (in
00204  * kT/e) at the specified point
00205  * @ingroup Vfetk
00206  * @author Nathan Baker
00207  * @param pbe Vpbe object
00208  * @param d Dimension of x
00209  * @param x Coordinates of point of interest (in &Aring;)
00210  * @note Thread-safe
00211  * @returns Multi-sphere Debye-Huckel potential in kT/e
00212  */
00213 VPRIVATE double debye_U(

```

```

00214         Vpbe *pbe,
00215         int d,
00216         double x[]
00217     );
00218
00219 /*
00220  * @brief Return the difference between the analytical multi-sphere
00221  * Debye-Huckel approximation and Coulomb's law (in kT/e) at the specified
00222  * point
00223  * @ingroup Vfetk
00224  * @author Nathan Baker
00225  * @param pbe Vpbe object
00226  * @param d Dimension of x
00227  * @param x Coordinates of point of interest (in &Aring;)
00228  * @note Thread-safe
00229  * @returns Multi-sphere Debye-Huckel potential in kT/e */
00230 VPRIVATE double debeye_Udiff(
00231     Vpbe *pbe,
00232     int d,
00233     double x[]
00234 );
00235
00236 /*
00237  * @brief Calculate the Coulomb's
00238  * Debye-Huckel approximation and Coulomb's law (in kT/e) at the specified
00239  * point
00240  * @ingroup Vfetk
00241  * @author Nathan Baker
00242  * @param pbe Vpbe object
00243  * @param d Dimension of x
00244  * @param x Coordinates of point of interest (in &Aring;)
00245  * @param eps Dielectric constant
00246  * @param U Set to potential (in kT/e)
00247  * @param dU Set to potential gradient (in kT/e/&Aring;)
00248  * @param d2U Set to Laplacian of potential (in \f$ kT e^{-1} \AA^{-2} \f$)
00249  * @returns Multi-sphere Debye-Huckel potential in kT/e */
00250 VPRIVATE void coulomb(
00251     Vpbe *pbe,
00252     int d,
00253     double x[],
00254     double eps,
00255     double *U,
00256     double dU[],
00257     double *d2U
00258 );
00259
00260 /*
00261  * @brief 2D linear master simplex information generator
00262  * @ingroup Vfetk
00263  * @author Mike Holst
00264  * @param dimIS dunno
00265  * @param ndof dunno
00266  * @param dof dunno
00267  * @param c dunno
00268  * @param cx dunno
00269  * @note Trust in Mike */
00270 VPRIVATE void init_2DP1(
00271     int dimIS[],
00272     int *ndof,
00273     int dof[],
00274     double c[][VMAXP],
00275     double cx[][VMAXP],
00276     double cy[][VMAXP],
00277     double cz[][VMAXP]
00278 );
00279
00280 /*
00281  * @brief 3D linear master simplex information generator
00282  * @ingroup Vfetk
00283  * @author Mike Holst
00284  * @param dimIS dunno
00285  * @param ndof dunno
00286  * @param dof dunno
00287  * @param c dunno
00288  * @param cx dunno
00289  * @param cy dunno
00290  * @param cz dunno
00291  * @note Trust in Mike */
00292 VPRIVATE void init_3DP1(
00293     int dimIS[],
00294     int *ndof,

```

```

00295         int dof[],
00296         double c[][VMAXP],
00297         double cx[][VMAXP],
00298         double cy[][VMAXP],
00299         double cz[][VMAXP]
00300     );
00301
00302 /*
00303  * @brief Setup coefficients of polynomials from integer table data
00304  * @ingroup Vfetk
00305  * @author Mike Holst
00306  * @param numP dunno
00307  * @param c dunno
00308  * @param cx dunno
00309  * @param cy dunno
00310  * @param cz dunno
00311  * @param ic dunno
00312  * @param icx dunno
00313  * @param icy dunno
00314  * @param icz dunno
00315  * @note Trust in Mike */
00316 VPRIVATE void setCoef(
00317     int numP,
00318     double c[][VMAXP],
00319     double cx[][VMAXP],
00320     double cy[][VMAXP],
00321     double cz[][VMAXP],
00322     int ic[][VMAXP],
00323     int icx[][VMAXP],
00324     int icy[][VMAXP],
00325     int icz[][VMAXP]
00326 );
00327
00328 /*
00329  * @brief Evaluate a collection of at most cubic polynomials at a
00330  * specified point in at most R^3.
00331  * @ingroup Vfetk
00332  * @author Mike Holst
00333  * @param numP the number of polynomials to evaluate
00334  * @param p the results of the evaluation
00335  * @param c the coefficients of each polynomial
00336  * @param xv the point (x,y,z) to evaluate the polynomials.
00337  * @note Mike says:
00338  * <pre>
00339  * Note that "VMAXP" must be >= 19 for cubic polynomials.
00340  * The polynomials are build from the coefficients c[][] as
00341  * follows. To build polynomial "k", fix k and set:
00342  *
00343  * c0=c[k][0], c1=c[k][1], .... , cp=c[k][p]
00344  *
00345  * Then evaluate as:
00346  *
00347  * p3(x,y,z) = c0 + c1*x + c2*y + c3*z
00348  *             + c4*x*x + c5*y*y + c6*z*z + c7*x*y + c8*x*z + c9*y*z
00349  *             + c10*x*x*x + c11*y*y*y + c12*z*z*z
00350  *             + c13*x*x*y + c14*x*x*z + c15*x*y*y
00351  *             + c16*y*y*z + c17*x*z*z + c18*y*z*z
00352  * </pre>
00353  */
00354 VPRIVATE void polyEval(
00355     int numP,
00356     double p[],
00357     double c[][VMAXP],
00358     double xv[]
00359 );
00360
00361 /*
00362  * @brief I have no clue what this variable does, but we need it to initialize
00363  * the simplices
00364  * @ingroup Vfetk
00365  * @author Mike Holst */
00366 VPRIVATE int dim_2DP1 = 3;
00367
00368 /*
00369  * @brief I have no clue what these variable do, but we need it to initialize
00370  * the simplices
00371  * @ingroup Vfetk
00372  * @author Mike Holst
00373  * @note Mike says:
00374  * <pre>
00375  * 2D-P1 Basis:

```

```

00376 *
00377 * p1(x,y) = c0 + c1*x + c2*y
00378 *
00379 * Lagrange Point      Lagrange Basis Function Definition
00380 * -----
00381 * (0, 0)              p[0](x,y) = 1 - x - y
00382 * (1, 0)              p[1](x,y) = x
00383 * (0, 1)              p[2](x,y) = y
00384 * </pre>
00385 */
00386 VPRIVATE int lgr_2DP1[3][VMAXP] = {
00387 /*c0 c1 c2 c3
00388 * ----- */
00389 /* 1 x y z
00390 * ----- */
00391 { 2, -2, -2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
00392 { 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
00393 { 0, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
00394 };
00395 VPRIVATE int lgr_2DP1x[3][VMAXP] = {
00396 /*c0
00397 /* 1
00398 { -2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
00399 { 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
00400 { 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
00401 };
00402 VPRIVATE int lgr_2DP1y[3][VMAXP] = {
00403 /*c0
00404 /* 1
00405 { -2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
00406 { 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
00407 { 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
00408 };
00409 VPRIVATE int lgr_2DP1z[3][VMAXP] = {
00410 /*c0
00411 /* 1
00412 { 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
00413 { 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
00414 { 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
00415 };
00416
00417
00418 /*
00419 * @brief I have no clue what these variable do, but we need it to initialize
00420 * the simplices
00421 * @ingroup Vfetk
00422 * @author Mike Holst
00423 * @note Mike says:
00424 * <pre>
00425 * 3D-P1 Basis:
00426 *
00427 * p1(x,y,z) = c0 + c1*x + c2*y + c3*z
00428 *
00429 * Lagrange Point      Lagrange Basis Function Definition
00430 * -----
00431 * (0, 0, 0)          p[0](x,y,z) = 1 - x - y - z
00432 * (1, 0, 0)          p[1](x,y,z) = x
00433 * (0, 1, 0)          p[2](x,y,z) = y
00434 * (0, 0, 1)          p[3](x,y,z) = z
00435 * </pre>
00436 */
00437 VPRIVATE int dim_3DP1 = VAPBS_NVS;
00438 VPRIVATE int lgr_3DP1[VAPBS_NVS][VMAXP] = {
00439 /*c0 c1 c2 c3
00440 /* 1 x y z
00441 { 2, -2, -2, -2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
00442 { 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
00443 { 0, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
00444 { 0, 0, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
00445 };
00446 VPRIVATE int lgr_3DP1x[VAPBS_NVS][VMAXP] = {
00447 /*c0
00448 /* 1
00449 { -2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
00450 { 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
00451 { 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
00452 { 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
00453 };
00454 VPRIVATE int lgr_3DP1y[VAPBS_NVS][VMAXP] = {
00455 /*c0
00456 /* 1

```

```

00457 { -2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
00458 { 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
00459 { 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
00460 { 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
00461 };
00462 VPRIVATE int lgr_3DP1z[VAPBS_NVS][VMAXP] = {
00463 /*c0 ----- */
00464 /* 1 ----- */
00465 { -2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
00466 { 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
00467 { 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
00468 { 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0 },
00469 };
00470
00471 /*
00472  * @brief Another Holst variable
00473  * @ingroup Vfetk
00474  * @author Mike Holst
00475  * @note Mike says: 1 = linear, 2 = quadratic */
00476 VPRIVATE const int P_DEG=1;
00477
00478 /*
00479  * @brief Another Holst variable
00480  * @ingroup Vfetk
00481  * @author Mike Holst */
00482 VPRIVATE int numP;
00483 VPRIVATE double c[VMAXP][VMAXP];
00484 VPRIVATE double cx[VMAXP][VMAXP];
00485 VPRIVATE double cy[VMAXP][VMAXP];
00486 VPRIVATE double cz[VMAXP][VMAXP];
00487
00488 #if !defined(VINLINE_VFETK)
00489
00490 VPUBLIC Gem* Vfetk_getGem(Vfetk *thee) {
00491
00492     VASSERT(thee != VNULL);
00493     return thee->gm;
00494 }
00495
00496
00497 VPUBLIC AM* Vfetk_getAM(Vfetk *thee) {
00498
00499     VASSERT(thee != VNULL);
00500     return thee->am;
00501 }
00502
00503 VPUBLIC Vpbe* Vfetk_getVpbe(Vfetk *thee) {
00504
00505     VASSERT(thee != VNULL);
00506     return thee->pbe;
00507 }
00508
00509
00510 VPUBLIC Vcsm* Vfetk_getVcsm(Vfetk *thee) {
00511
00512     VASSERT(thee != VNULL);
00513     return thee->csm;
00514 }
00515
00516
00517 VPUBLIC int Vfetk_getAtomColor(Vfetk *thee,
00518                               int iatom
00519                               ) {
00520
00521     int natoms;
00522
00523     VASSERT(thee != VNULL);
00524
00525     natoms = Valist_getNumberAtoms(Vpbe_getValist(thee->pbe));
00526     VASSERT(iatom < natoms);
00527
00528     return Vatom_getPartID(Valist_getAtom(Vpbe_getValist(thee->pbe), iatom));
00529 }
00530 #endif /* if !defined(VINLINE_VFETK) */
00531
00532 VPUBLIC Vfetk* Vfetk_ctor(Vpbe *pbe,
00533                          Vhal_PBEType type
00534                          ) {
00535
00536     /* Set up the structure */
00537     Vfetk *thee = VNULL;

```



```

00538     thee = (Vfetk*)Vmem_malloc(VNULL, 1, sizeof(Vfetk) );
00539     VASSERT(thee != VNULL);
00540     VASSERT(Vfetk_ctor2(thee, pbe, type));
00541
00542     return thee;
00543 }
00544
00545 VPUBLIC int Vfetk_ctor2(Vfetk *thee,
00546                        Vpbe *pbe,
00547                        Vhal_PBEType type
00548                        ) {
00549
00550     int i;
00551     double center[VAPBS_DIM];
00552
00553     /* Make sure things have been properly initialized & store them */
00554     VASSERT(pbe != VNULL);
00555     thee->pbe = pbe;
00556     VASSERT(pbe->alist != VNULL);
00557     VASSERT(pbe->acc != VNULL);
00558
00559     /* Store PBE type */
00560     thee->type = type;
00561
00562     /* Set up memory management object */
00563     thee->vmem = Vmem_ctor("APBS::VFETK");
00564
00565     /* Set up FEtk objects */
00566     Vnm_print(0, "Vfetk_ctor2: Constructing PDE...\n");
00567     thee->pde = Vfetk_PDE_ctor(thee);
00568     Vnm_print(0, "Vfetk_ctor2: Constructing Gem...\n");
00569     thee->gm = Gem_ctor(thee->vmem, thee->pde);
00570     Vnm_print(0, "Vfetk_ctor2: Constructing Aprx...\n");
00571     thee->aprx = Aprx_ctor(thee->vmem, thee->gm, thee->pde);
00572     Vnm_print(0, "Vfetk_ctor2: Constructing Aprx...\n");
00573     thee->am = AM_ctor(thee->vmem, thee->aprx);
00574
00575     /* Reset refinement level */
00576     thee->level = 0;
00577
00578     /* Set default solver variables */
00579     thee->lkey = VLT_MG;
00580     thee->lmax = 1000000;
00581     thee->ltol = 1e-5;
00582     thee->lprec = VPT_MG;
00583     thee->nkey = VNT_NEW;
00584     thee->nmax = 1000000;
00585     thee->ntol = 1e-5;
00586     thee->gues = VGT_ZERO;
00587     thee->pjac = -1;
00588
00589     /* Store local copy of myself */
00590     var.fetk = thee;
00591     var.initGreen = 0;
00592
00593     /* Set up the external Gem subdivision hook */
00594     Gem_setExternalUpdateFunction(thee->gm, Vfetk_externalUpdateFunction);
00595
00596     /* Set up ion-related variables */
00597     var.zkappa2 = Vpbe_getZkappa2(var.fetk->pbe);
00598     var.ionstr = Vpbe_getBulkIonicStrength(var.fetk->pbe);
00599     if (var.ionstr > 0.0) var.zks2 = 0.5*var.zkappa2/var.ionstr;
00600     else var.zks2 = 0.0;
00601     Vpbe_getIons(var.fetk->pbe, &(var.nion), var.ionConc, var.ionRadii,
00602                 var.ionQ);
00603     for (i=0; i<var.nion; i++) {
00604         var.ionConc[i] = var.zks2 * var.ionConc[i] * var.ionQ[i];
00605     }
00606
00607     /* Set uninitialized objects to NULL */
00608     thee->pbeparm = VNULL;
00609     thee->feparm = VNULL;
00610     thee->csm = VNULL;
00611
00612     return 1;
00613 }
00614
00615 VPUBLIC void Vfetk_setParameters(Vfetk *thee,
00616                                PBEParm *pbeparm,
00617                                FEMparm *feparm
00618                                ) {

```

```

00619
00620     VASSERT(thee != VNULL);
00621     thee->feparm = feparm;
00622     thee->pbeparm = pbeparm;
00623 }
00624
00625 VPUBLIC void Vfetc_dtor(Vfetc **thee) {
00626     if ((*thee) != VNULL) {
00627         Vfetc_dtor2(*thee);
00628         //Vmem_free(VNULL, 1, sizeof(Vfetc), (void **)thee);
00629         (*thee) = VNULL;
00630     }
00631 }
00632
00633 VPUBLIC void Vfetc_dtor2(Vfetc *thee) {
00634     Vcsm_dtor(&(thee->csm));
00635     AM_dtor(&(thee->am));
00636     Aprx_dtor(&(thee->apr));
00637     Vfetc_PDE_dtor(&(thee->pde));
00638     Vmem_dtor(&(thee->vmem));
00639 }
00640
00641 VPUBLIC double* Vfetc_getSolution(Vfetc *thee,
00642                                 int *length
00643                                 ) {
00644
00645     int i;
00646     double *solution,
00647           *theAnswer;
00648     AM *am;
00649
00650     VASSERT(thee != VNULL);
00651
00652     /* Get the AM object */
00653     am = thee->am;
00654     /* Copy the solution into the w0 vector */
00655     Bvec_copy(am->w0, am->u);
00656     /* Add the Dirichlet conditions */
00657     Bvec_axpy(am->w0, am->ud, 1.);
00658     /* Get the data from the Bvec */
00659     solution = Bvec_addr(am->w0);
00660     /* Get the length of the data from the Bvec */
00661     *length = Bvec_numRT(am->w0);
00662     /* Make sure that we got scalar data (only one block) for the solution
00663      * to the FETK */
00664     VASSERT(1 == Bvec_numB(am->w0));
00665     /* Allocate space for the returned vector and copy the solution into it */
00666     theAnswer = VNULL;
00667     theAnswer = (double*)Vmem_malloc(VNULL, *length, sizeof(double));
00668     VASSERT(theAnswer != VNULL);
00669     for (i=0; i<(*length); i++) theAnswer[i] = solution[i];
00670
00671     return theAnswer;
00672 }
00673
00674
00693 VPUBLIC double Vfetc_energy(Vfetc *thee,
00694                             int color,
00695                             int nonlin
00700                             ) {
00701
00702     double totEnergy = 0.0,
00703           qfEnergy = 0.0,
00704           dqmEnergy = 0.0;
00705     VASSERT(thee != VNULL);
00706
00707     if (nonlin && (Vpbe_getBulkIonicStrength(thee->pbe) > 0.)) {
00708         Vnm_print(0, "Vfetc_energy: calculating full PBE energy\n");
00709         Vnm_print(0, "Vfetc_energy: bulk ionic strength = %g M\n",
00710                 Vpbe_getBulkIonicStrength(thee->pbe));
00711         dqmEnergy = Vfetc_dqmEnergy(thee, color);
00712         Vnm_print(0, "Vfetc_energy: dqmEnergy = %g kT\n", dqmEnergy);
00713         qfEnergy = Vfetc_qfEnergy(thee, color);
00714         Vnm_print(0, "Vfetc_energy: qfEnergy = %g kT\n", qfEnergy);
00715
00716         totEnergy = qfEnergy - dqmEnergy;
00717     } else {
00718         Vnm_print(0, "Vfetc_energy: calculating only q-phi energy\n");
00719         dqmEnergy = Vfetc_dqmEnergy(thee, color);
00720         Vnm_print(0, "Vfetc_energy: dqmEnergy = %g kT (NOT USED)\n", dqmEnergy);
00721         qfEnergy = Vfetc_qfEnergy(thee, color);
00722     }

```

```

00723         Vnm_print(0, "Vfetk_energy:  qfEnergy = %g kT\n", qfEnergy);
00724         totEnergy = 0.5*qfEnergy;
00725     }
00726
00727     return totEnergy;
00728
00729 }
00730
00731
00732 VPUBLIC double Vfetk_qfEnergy(Vfetk *thee,
00733                             int color
00734                             ) {
00735
00736     double *sol,
00737           energy = 0.0;
00738     int nsol,
00739         iatom,
00740         natoms;
00741     AM *am;
00742
00743     VASSERT(thee != VNULL);
00744     am = thee->am;
00745
00746     /* Get the finest level solution */
00747     sol= VNULL;
00748     sol = Vfetk_getSolution(thee, &nsol);
00749     VASSERT(sol != VNULL);
00750
00751     /* Make sure the number of entries in the solution array matches the
00752      * number of vertices currently in the mesh */
00753     if (nsol != Gem_numVV(thee->gm)) {
00754         Vnm_print(2, "Vfetk_qfEnergy: Number of unknowns in solution does not match\n");
00755         Vnm_print(2, "Vfetk_qfEnergy: number of vertices in mesh!!!  Bailing out!\n");
00756         VASSERT(0);
00757     }
00758
00759     /* Now we do the sum over atoms... */
00760     natoms = Valist_getNumberAtoms(thee->pbe->alist);
00761     for (iatom=0; iatom<natoms; iatom++) {
00762
00763         energy = energy + Vfetk_qfEnergyAtom(thee, iatom, color, sol);
00764
00765     } /* end for iatom */
00766
00767     /* Destroy the finest level solution */
00768     Vmem_free(VNULL, nsol, sizeof(double), (void **)&sol);
00769
00770     /* Return the energy */
00771     return energy;
00772 }
00773
00774 VPRIVATE double Vfetk_qfEnergyAtom(
00775     Vfetk *thee,
00776     int iatom,
00777     int color,
00778     double *sol) {
00779
00780     Vatom *atom;
00781     double charge,
00782           phi[VAPBS_NVS],
00783           phix[VAPBS_NVS][3],
00784           *position,
00785           uval,
00786           energy = 0.0;
00787     int isimp,
00788         nsimps,
00789         icolor,
00790         invert,
00791         usingColor;
00792     SS *simp;
00793
00794
00795     /* Get atom information */
00796     atom = Valist_getAtom(thee->pbe->alist, iatom);
00797     icolor = Vfetk_getAtomColor(thee, iatom);
00798     charge = Vatom_getCharge(atom);
00799     position = Vatom_getPosition(atom);
00800
00801     /* Find out if we're using colors */
00802     usingColor = (color >= 0);
00803

```

```

00804     if (usingColor && (icolor<0)) {
00805         Vnm_print(2, "Vfetk_qfEnergy: Atom colors not set!\n");
00806         VASSERT(0);
00807     }
00808
00809     /* Check if this atom belongs to the specified partition */
00810     if ((icolor==color) || (!usingColor)) {
00811         /* Loop over the sims associated with this atom */
00812         nsimps = Vcsm_getNumberSimplices(thee->csm, iatom);
00813
00814         /* Get the first simp of the correct color; we can use just one
00815          * simplex for energy evaluations, but not for force
00816          * evaluations */
00817         for (isimp=0; isimp<nsimps; isimp++) {
00818
00819             simp = Vcsm_getSimplex(thee->csm, isimp, iatom);
00820
00821             /* If we've asked for a particular partition AND if the atom
00822              * is our partition, then compute the energy */
00823             if ((SS_chart(simp)==color) || (color<0)) {
00824                 /* Get the value of each basis function evaluated at this
00825                  * point */
00826                 Gem_pointInSimplexVal(thee->gm, simp, position, phi, phix);
00827                 for (ivert=0; ivert<SS_dimVV(simp); ivert++) {
00828                     uval = sol[VV_id(SS_vertex(simp,ivert))];
00829                     energy += (charge*phi[ivert]*uval);
00830                 } /* end for ivert */
00831                 /* We only use one simplex of the appropriate color for
00832                  * energy calculations, so break here */
00833                 break;
00834             } /* endif (color) */
00835         } /* end for isimp */
00836     }
00837
00838     return energy;
00839 }
00840
00841
00842 VPUBLIC double Vfetk_dqmEnergy(Vfetk *thee,
00843                               int color) {
00844
00845     return AM_evalJ(thee->am);
00846 }
00847
00848
00849 VPUBLIC void Vfetk_setAtomColors(Vfetk *thee) {
00850
00851     SS *simp;
00852     Vatom *atom;
00853     int i,
00854         natoms;
00855
00856     VASSERT(thee != VNULL);
00857
00858     natoms = Valist_getNumberAtoms(thee->pbe->alist);
00859     for (i=0; i<natoms; i++) {
00860         atom = Valist_getAtom(thee->pbe->alist, i);
00861         simp = Vcsm_getSimplex(thee->csm, 0, i);
00862         Vatom_setPartID(atom, SS_chart(simp));
00863     }
00864 }
00865
00866
00867 VPUBLIC unsigned long int Vfetk_memChk(Vfetk *thee) {
00868
00869     int memUse = 0;
00870
00871     if (thee == VNULL) return 0;
00872
00873     memUse = memUse + sizeof(Vfetk);
00874     memUse = memUse + Vcsm_memChk(thee->csm);
00875
00876     return memUse;
00877 }
00878
00885 VPUBLIC Vrc_Codes Vfetk_genCube(Vfetk *thee,
00886                                double center[3],
00887                                double length[3],
00888                                Vfetk_MeshLoad meshType
00889                                ) {
00890

```

```

00891     VASSERT(thee != VNULL);
00892
00893     AM *am = VNULL; /* @todo - no idea what this is */
00894     Gem *gm = VNULL; /* Geometry manager */
00895
00896     int skey = 0, /* Simplex format */
00897         bufsize = 0, /* Buffer size */
00898         i, /* Loop counter */
00899         j; /* Loop counter */
00900     char *key = "r", /* Read */
00901         *iodev = "BUFF", /* Buffer */
00902         *iofmt = "ASC", /* ASCII */
00903         *iohost = "localhost", /* localhost (dummy) */
00904         *iofile = "0", /*< socket 0 (dummy) */
00905         buf[VMAX_BUFSIZE]; /* Socket buffer */
00906     Vio *sock = VNULL; /* Socket object */
00907     VV *vx = VNULL; /* @todo - no idea what this is */
00908     double x;
00909
00910     am = thee->am;
00911     VASSERT(am != VNULL);
00912     gm = thee->gm;
00913     VASSERT(gm != VNULL);
00914
00915     /* @note This code is based on Gem_makeCube by Mike Holst */
00916     /* Write mesh string to buffer and read back */
00917     switch (meshType) {
00918     case VML_DIRICUBE:
00919         /* Create a new copy of the DIRICUBE mesh (see globals higher in this file) */
00920         bufsize = strlen(diriCubeString);
00921         VASSERT( bufsize <= VMAX_BUFSIZE );
00922         strncpy(buf, diriCubeString, VMAX_BUFSIZE);
00923         break;
00924     case VML_NEUMCUBE:
00925         /* Create a new copy of the NEUMCUBE mesh (see globals higher in this file) */
00926         bufsize = strlen(neumCubeString);
00927         Vnm_print(2, "Vfetk_genCube: WARNING! USING EXPERIMENTAL NEUMANN BOUNDARY CONDITIONS!\n");
00928         VASSERT( bufsize <= VMAX_BUFSIZE );
00929         strncpy(buf, neumCubeString, VMAX_BUFSIZE);
00930         break;
00931     case VML_EXTERNAL:
00932         Vnm_print(2, "Vfetk_genCube: Got request for external mesh!\n");
00933         Vnm_print(2, "Vfetk_genCube: How did we get here?\n");
00934         return VRC_FAILURE;
00935     default:
00936         Vnm_print(2, "Vfetk_genCube: Unknown mesh type (%d)\n", meshType);
00937         return VRC_FAILURE;
00938     }
00939
00940     VASSERT( VNULL != (sock=Vio_socketOpen(key,iodev,iofmt,iohost,iofile)) ); /* Open socket */
00941     Vio_bufTake(sock, buf, bufsize); /* Initialize internal buffer for socket */
00942     AM_read(am, skey, sock); /* Take the initial mesh from the socket and load
00943                               into internal AM data structure with simplex
00944                               format */
00945     Vio_connectFree(sock); /* Purge output buffers */
00946     Vio_bufGive(sock); /* Get pointer to output buffer? No assignment of return value... */
00947     Vio_dtor(&sock); /* Destroy output buffer */
00948
00949     /* @todo - could the following be done in a single pass? - PCE */
00950     /* Scale (unit) cube - for each vertex, set the new coordinates of that
00951        vertex based on the vertex length */
00952     for (i=0; i<Gem_numVV(gm); i++) {
00953         vx = Gem_VV(gm, i);
00954         for (j=0; j<3; j++) {
00955             x = VV_coord(vx, j);
00956             x *= length[j];
00957             VV_setCoord(vx, j, x);
00958         }
00959     }
00960
00961     /* Add new center - for each vertex, set a new center for the vertex */
00962     for (i=0; i<Gem_numVV(gm); i++) {
00963         vx = Gem_VV(gm, i);
00964         for (j=0; j<3; j++) {
00965             x = VV_coord(vx, j);
00966             x += center[j];
00967             VV_setCoord(vx, j, x);
00968         }
00969     }
00970
00971     return VRC_SUCCESS;

```

```

00972 }
00973
00980 VPUBLIC Vrc_Codes Vfetk_loadMesh(Vfetk *thee, /* Vfetk object to load into */
00981                                double center[3], /* Center for mesh (if constructed) */
00982                                double length[3], /* Mesh lengths (if constructed) */
00983                                Vfetk_MeshLoad meshType, /* Type of mesh to load */
00984                                Vio *sock /* Socket for external mesh data (NULL otherwise) */
00985                                ) {
00986
00987     Vrc_Codes vrc; /* Function return codes - see vhal.h for enum */
00988     int skey = 0; /* Simplex format */
00989
00990     /* Load mesh from socket if external mesh, otherwise generate mesh */
00991     switch (meshType) {
00992     case VML_EXTERNAL:
00993         if (sock == VNULL) {
00994             Vnm_print(2, "Vfetk_loadMesh: Got NULL socket!\n");
00995             return VRC_FAILURE;
00996         }
00997         AM_read(thee->am, skey, sock);
00998         Vio_connectFree(sock);
00999         Vio_bufGive(sock);
01000         Vio_dtor(&sock);
01001         break;
01002     case VML_DIRICUBE:
01003     case VML_NEUMCUBE:
01004         /* Create new mesh and store in thee */
01005         vrc = Vfetk_genCube(thee, center, length, meshType);
01006         if (vrc == VRC_FAILURE) return VRC_FAILURE;
01007         break;
01008     default:
01009         Vnm_print(2, "Vfetk_loadMesh: unrecognized mesh type (%d)!\n",
01010                 meshType);
01011         return VRC_FAILURE;
01012     };
01013
01014     /* Setup charge-simplex map */
01015     Vnm_print(0, "Vfetk_ctor2: Constructing Vcsm...\n");
01016     thee->csm = VNULL;
01017     /* Construct a new Vcsm with the atom list and gem data */
01018     thee->csm = Vcsm_ctor(Vpbe_getValist(thee->pbe), thee->gm);
01019     VASSERT(thee->csm != VNULL);
01020     Vcsm_init(thee->csm);
01021
01022     return VRC_SUCCESS;
01023 }
01024
01025
01026 VPUBLIC void Bmat_printHB(Bmat *thee,
01027                          char *fname
01028                          ) {
01029
01030     Mat *Ablock;
01031     MATsym pqsym;
01032     int i, j, jj;
01033     int *IA, *JA;
01034     double *D, *L, *U;
01035     FILE *fp;
01036
01037     char mmttitle[72];
01038     char mmkey[] = {"8charkey"};
01039     int totc = 0, ptrc = 0, indc = 0, valc = 0;
01040     char mxtyp[] = {"RUA"}; /* Real Unsymmetric Assembled */
01041     int nrow = 0, ncol = 0, numZ = 0;
01042     int numZdigits = 0, nrowdigits = 0;
01043     int nprline = 8, nindline = 8, nvalline = 5;
01044     char ptrfmt[] = {"(8I10)", ptrfmtstr[] = {"%10d"};
01045     char indfmt[] = {"(8I10)", indfmtstr[] = {"%10d"};
01046     char valfmt[] = {"(5E16.8)", valfmtstr[] = {"%16.8E"};
01047
01048     VASSERT( thee->numB == 1 ); /* HARDWARE FOR NOW */
01049     Ablock = thee->AD[0][0];
01050
01051     VASSERT( Mat_format( Ablock ) == DRC_FORMAT ); /* HARDWARE FOR NOW */
01052
01053     pqsym = Mat_sym( Ablock );
01054
01055     if ( pqsym == IS_SYM ) {
01056         mxtyp[1] = 'S';
01057     } else if ( pqsym == ISNOT_SYM ) {
01058         mxtyp[1] = 'U';

```

```

01059     } else {
01060         VASSERT( 0 ); /* NOT VALID */
01061     }
01062
01063     nrow = Bmat_numRT( thee ); /* Number of rows */
01064     ncol = Bmat_numCT( thee ); /* Number of cols */
01065     numZ = Bmat_numZT( thee ); /* Number of entries */
01066
01067     nrowdigits = (int) (log( nrow )/log( 10 )) + 1;
01068     numZdigits = (int) (log( numZ )/log( 10 )) + 1;
01069
01070     nptrline = (int) ( 80 / (numZdigits + 1) );
01071     nindline = (int) ( 80 / (nrowdigits + 1) );
01072
01073     sprintf(ptrfmt,"%dI%d",nptrline,numZdigits+1);
01074     sprintf(ptrfmtstr,"%%dd",numZdigits+1);
01075     sprintf(indfmt,"%dI%d",nindline,nrowdigits+1);
01076     sprintf(indfmtstr,"%%dd",nrowdigits+1);
01077
01078     ptrc = (int) ( ( ncol + 1 ) - 1 ) / nptrline ) + 1;
01079     indc = (int) ( ( numZ - 1 ) / nindline ) + 1;
01080     valc = (int) ( ( numZ - 1 ) / nvalline ) + 1;
01081
01082     totc = ptrc + indc + valc;
01083
01084     sprintf( mmtitle, "Sparse '%s' Matrix - Harwell-Boeing Format - '%s'",
01085             thee->name, fname );
01086
01087     /* Step 0: Open the file for writing */
01088
01089     fp = fopen( fname, "w" );
01090     if (fp == VNULL) {
01091         Vnm_print(2,"Bmat_printHB: Ouch couldn't open file <%s>\n",fname);
01092         return;
01093     }
01094
01095     /* Step 1: Print the header information */
01096
01097     fprintf( fp, "%-72s%-8s\n", mmtitle, mmkey );
01098     fprintf( fp, "%14d%14d%14d%14d%14d\n", totc, ptrc, indc, valc, 0 );
01099     fprintf( fp, "%3s%11s%14d%14d%14d\n", mxtyp, " ", nrow, ncol, numZ );
01100     fprintf( fp, "%-16s%-16s%-20s%-20s\n", ptrfmt, indfmt, valfmt, "6E13.5" );
01101
01102     IA = Ablock->IA;
01103     JA = Ablock->JA;
01104     D = Ablock->diag;
01105     L = Ablock->offL;
01106     U = Ablock->offU;
01107
01108     if ( pqsym == IS_SYM ) {
01109
01110         /* Step 2: Print the pointer information */
01111
01112         for (i=0; i<(ncol+1); i++) {
01113             fprintf( fp, ptrfmtstr, Ablock->IA[i] + (i+1) );
01114             if ( ( i+1 ) % nptrline ) == 0 ) {
01115                 fprintf( fp, "\n" );
01116             }
01117         }
01118
01119         if ( ( ( ncol+1 ) % nptrline ) != 0 ) {
01120             fprintf( fp, "\n" );
01121         }
01122
01123         /* Step 3: Print the index information */
01124
01125         j = 0;
01126         for (i=0; i<ncol; i++) {
01127             fprintf( fp, indfmtstr, i+1); /* diagonal */
01128             if ( ( (j+1) % nindline ) == 0 ) {
01129                 fprintf( fp, "\n" );
01130             }
01131             j++;
01132             for (jj=IA[i]; jj<IA[i+1]; jj++) {
01133                 fprintf( fp, indfmtstr, JA[jj] + 1 ); /* lower triangle */
01134                 if ( ( (j+1) % nindline ) == 0 ) {
01135                     fprintf( fp, "\n" );
01136                 }
01137             }
01138             j++;
01139         }

```

```

01140
01141     if ( ( j % nindline ) != 0 ) {
01142         fprintf( fp, "\n" );
01143     }
01144
01145     /* Step 4: Print the value information */
01146
01147     j = 0;
01148     for (i=0; i<ncol; i++) {
01149         fprintf( fp, valfmtstr, D[i] );
01150         if ( ( (j+1) % nvalline ) == 0 ) {
01151             fprintf( fp, "\n" );
01152         }
01153         j++;
01154         for (jj=IA[i]; jj<IA[i+1]; jj++) {
01155             fprintf( fp, valfmtstr, L[jj] );
01156             if ( ( (j+1) % nvalline ) == 0 ) {
01157                 fprintf( fp, "\n" );
01158             }
01159             j++;
01160         }
01161     }
01162
01163     if ( ( j % nvalline ) != 0 ) {
01164         fprintf( fp, "\n" );
01165     }
01166
01167 } else { /* ISNOT_SYM */
01168
01169     VASSERT( 0 ); /* NOT CODED YET */
01170 }
01171
01172 /* Step 5: Close the file */
01173 fclose( fp );
01174 }
01175
01176 VPUBLIC PDE* Vfetk_PDE_ctor(Vfetk *fetk) {
01177
01178     PDE *thee = VNULL;
01179
01180     thee = (PDE*)Vmem_malloc(fetk->vmem, 1, sizeof(PDE));
01181     VASSERT(thee != VNULL);
01182     VASSERT(Vfetk_PDE_ctor2(thee, fetk));
01183
01184     return thee;
01185 }
01186
01187 VPUBLIC int Vfetk_PDE_ctor2(PDE *thee,
01188                             Vfetk *fetk
01189                             ) {
01190
01191     int i;
01192
01193     if (thee == VNULL) {
01194         Vnm_print(2, "Vfetk_PDE_ctor2: Got NULL thee!\n");
01195         return 0;
01196     }
01197
01198     /* Store a local copy of the Vfetk class */
01199     var.fetk = fetk;
01200
01201     /* PDE-specific parameters and function pointers */
01202     thee->initAssemble = Vfetk_PDE_initAssemble;
01203     thee->initElement  = Vfetk_PDE_initElement;
01204     thee->initFace     = Vfetk_PDE_initFace;
01205     thee->initPoint    = Vfetk_PDE_initPoint;
01206     thee->Fu           = Vfetk_PDE_Fu;
01207     thee->Fu_v         = Vfetk_PDE_Fu_v;
01208     thee->DFu_wv       = Vfetk_PDE_DFu_wv;
01209     thee->delta        = Vfetk_PDE_delta;
01210     thee->u_D          = Vfetk_PDE_u_D;
01211     thee->u_T          = Vfetk_PDE_u_T;
01212     thee->Ju           = Vfetk_PDE_Ju;
01213     thee->vec          = 1; /* FIX! */
01214     thee->sym[0][0]    = 1;
01215     thee->est[0]       = 1.0;
01216     for (i=0; i<VMAX_BDTYPE; i++) thee->bmap[0][i] = i;
01217
01218     /* Manifold-specific function pointers */
01219     thee->bisectEdge    = Vfetk_PDE_bisectEdge;
01220     thee->mapBoundary  = Vfetk_PDE_mapBoundary;

```



```

01221     thee->markSimplex = Vfetk_PDE_markSimplex;
01222     thee->oneChart     = Vfetk_PDE_oneChart;
01223
01224     /* Element-specific function pointers */
01225     thee->simplexBasisInit = Vfetk_PDE_simplexBasisInit;
01226     thee->simplexBasisForm = Vfetk_PDE_simplexBasisForm;
01227
01228     return 1;
01229 }
01230
01231 VPUBLIC void Vfetk_PDE_dtor(PDE **thee) {
01232
01233     if ((*thee) != VNULL) {
01234         Vfetk_PDE_dtor2(*thee);
01235         /* TODO: The following line is commented out because at the moment,
01236            there is a seg fault when deallocating at the end of a run. Since
01237            this routine is called only once at the very end, we'll leave it
01238            commented out. However, this could be a memory leak.
01239            */
01240         /* Vmem_free(var.fetk->vmem, 1, sizeof(PDE), (void **)thee); */
01241         (*thee) = VNULL;
01242     }
01243 }
01244
01245 VPUBLIC void Vfetk_PDE_dtor2(PDE *thee) {
01246     var.fetk = VNULL;
01247 }
01248
01249 VPRIVATE double smooth(int nverts, double dist[VAPBS_NVS], double coeff[VAPBS_NVS], int meth) {
01250
01251     int i;
01252     double weight;
01253     double num = 0.0;
01254     double den = 0.0;
01255
01256     for (i=0; i<nverts; i++) {
01257         if (dist[i] < VSMALL) return coeff[i];
01258         weight = 1.0/dist[i];
01259         if (meth == 0) {
01260             num += (weight * coeff[i]);
01261             den += weight;
01262         } else if (meth == 1) {
01263             /* Small coefficients reset the average to 0; we need to break out
01264                * of the loop */
01265             if (coeff[i] < VSMALL) {
01266                 num = 0.0;
01267                 break;
01268             } else {
01269                 num += weight; den += (weight/coeff[i]);
01270             }
01271         } else VASSERT(0);
01272     }
01273
01274     return (num/den);
01275 }
01276
01277 }
01278
01279 VPRIVATE double diel() {
01280
01281     int i, j;
01282     double epsp, epsw, dist[5], coeff[5], srاد, swin, *vx;
01283     Vsurf_Meth srfm;
01284     Vacc *acc;
01285     PBEParm *pbeparm;
01286
01287     epsp = Vpbe_getSoluteDiel(var.fetk->pbe);
01288     epsw = Vpbe_getSolventDiel(var.fetk->pbe);
01289     VASSERT(var.fetk->pbeparm != VNULL);
01290     pbeparm = var.fetk->pbeparm;
01291     srfm = pbeparm->srfm;
01292     srاد = pbeparm->srاد;
01293     swin = pbeparm->swin;
01294     acc = var.fetk->pbe->acc;
01295
01296     eps = 0;
01297
01298     if (VABS(epsp - epsw) < VSMALL) return epsp;
01299     switch (srfm) {
01300     case VSM_MOL:
01301         eps = ((epsw-epsp)*Vacc_molAcc(acc, var.xq, srاد) + epsp);

```

```

01302         break;
01303     case VSM_MOLSMOOTH:
01304         for (i=0; i<var.nverts; i++) {
01305             dist[i] = 0;
01306             vx = var.vx[i];
01307             for (j=0; j<3; j++) {
01308                 dist[i] += VSQR(var.xq[j] - vx[j]);
01309             }
01310             dist[i] = VSQRT(dist[i]);
01311             coeff[i] = (epsw-epsp)*Vacc_molAcc(acc, var.xq, srad) + epsp;
01312         }
01313         eps = smooth(var.nverts, dist, coeff, 1);
01314         break;
01315     case VSM_SPLINE:
01316         eps = ((epsw-epsp)*Vacc_splineAcc(acc, var.xq, swin, 0.0) + epsp);
01317         break;
01318     default:
01319         Vnm_print(2, "Undefined surface method (%d)!\n", srfm);
01320         VASSERT(0);
01321     }
01322 }
01323 return eps;
01324 }
01325
01326 VPRIVATE double ionacc() {
01327     int i, j;
01328     double dist[5], coeff[5], irad, swin, *vx, accval;
01329     Vsurf_Meth srfm;
01330     Vacc *acc = VNULL;
01331     PBEparm *pbeparm = VNULL;
01332
01333     VASSERT(var.fetk->pbeparm != VNULL);
01334     pbeparm = var.fetk->pbeparm;
01335     srfm = pbeparm->srfm;
01336     irad = Vpbe_getMaxIonRadius(var.fetk->pbe);
01337     swin = pbeparm->swin;
01338     acc = var.fetk->pbe->acc;
01339
01340     if (var.zks2 < VSMALL) return 0.0;
01341     switch (srfm) {
01342     case VSM_MOL:
01343         accval = Vacc_ivdwAcc(acc, var.xq, irad);
01344         break;
01345     case VSM_MOLSMOOTH:
01346         for (i=0; i<var.nverts; i++) {
01347             dist[i] = 0;
01348             vx = var.vx[i];
01349             for (j=0; j<3; j++) {
01350                 dist[i] += VSQR(var.xq[j] - vx[j]);
01351             }
01352             dist[i] = VSQRT(dist[i]);
01353             coeff[i] = Vacc_ivdwAcc(acc, var.xq, irad);
01354         }
01355         accval = smooth(var.nverts, dist, coeff, 1);
01356         break;
01357     case VSM_SPLINE:
01358         accval = Vacc_splineAcc(acc, var.xq, swin, irad);
01359         break;
01360     default:
01361         Vnm_print(2, "Undefined surface method (%d)!\n", srfm);
01362         VASSERT(0);
01363     }
01364 }
01365
01366 return accval;
01367 }
01368
01369 VPRIVATE double debye_U(Vpbe *pbe, int d, double x[]) {
01370     double size, *position, charge, xkappa, eps_w, dist, T, pot, val;
01371     int iatom, i;
01372     Valist *alist;
01373     Vatom *atom;
01374
01375     eps_w = Vpbe_getSolventDiel(pbe);
01376     xkappa = (1.0e10)*Vpbe_getXkappa(pbe);
01377     T = Vpbe_getTemperature(pbe);
01378     alist = Vpbe_getValist(pbe);
01379     val = 0;
01380     pot = 0;

```

```

01383     for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
01384         atom = Valist_getAtom(alist, iatom);
01385         position = Vatom_getPosition(atom);
01386         charge = Vunit_ec*Vatom_getCharge(atom);
01387         size = (1e-10)*Vatom_getRadius(atom);
01388         dist = 0;
01389         for (i=0; i<d; i++) {
01390             dist += VSQR(position[i] - x[i]);
01391         }
01392         dist = (1.0e-10)*VSQRT(dist);
01393         val = (charge)/(4*VPI*Vunit_eps0*eps_w*dist);
01394         if (xkappa != 0.0) {
01395             val = val*(exp(-xkappa*(dist-size))/(1+xkappa*size));
01396         }
01397         pot = pot + val;
01398     }
01399     pot = pot*Vunit_ec/(Vunit_kb*T);
01400
01401     return pot;
01402 }
01403
01404 VPRIVATE double debye_Udiff(Vpbe *pbe, int d, double x[]) {
01405
01406     double size, *position, charge, eps_p, dist, T, pot, val;
01407     double Ufull;
01408     int iatom, i;
01409     Valist *alist;
01410     Vatom *atom;
01411
01412     Ufull = debye_U(pbe, d, x);
01413
01414     eps_p = Vpbe_getSoluteDiel(pbe);
01415     T = Vpbe_getTemperature(pbe);
01416     alist = Vpbe_getValist(pbe);
01417     val = 0;
01418     pot = 0;
01419
01420     for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
01421         atom = Valist_getAtom(alist, iatom);
01422         position = Vatom_getPosition(atom);
01423         charge = Vunit_ec*Vatom_getCharge(atom);
01424         size = (1e-10)*Vatom_getRadius(atom);
01425         dist = 0;
01426         for (i=0; i<d; i++) {
01427             dist += VSQR(position[i] - x[i]);
01428         }
01429         dist = (1.0e-10)*VSQRT(dist);
01430         val = (charge)/(4*VPI*Vunit_eps0*eps_p*dist);
01431         pot = pot + val;
01432     }
01433     pot = pot*Vunit_ec/(Vunit_kb*T);
01434
01435     pot = Ufull - pot;
01436
01437     return pot;
01438 }
01439
01440 VPRIVATE void coulomb(Vpbe *pbe, int d, double pt[], double eps, double *U,
01441     double dU[], double *d2U) {
01442
01443     int iatom, i;
01444     double T, pot, fx, fy, fz, x, y, z, scale;
01445     double *position, charge, dist, dist2, val, vec[3], dUold[3], Uold;
01446     Valist *alist;
01447     Vatom *atom;
01448
01449     /* Initialize variables */
01450     T = Vpbe_getTemperature(pbe);
01451     alist = Vpbe_getValist(pbe);
01452     pot = 0; fx = 0; fy = 0; fz = 0;
01453     x = pt[0]; y = pt[1]; z = pt[2];
01454
01455     /* Calculate */
01456     if (!Vgreen_coulombD(var.green, 1, &x, &y, &z, &pot, &fx, &fy, &fz)) {
01457         Vnm_print(2, "Error calculating Green's function!\n");
01458         VASSERT(0);
01459     }
01460
01461     /* Scale the results */
01462     scale = Vunit_ec/(eps*Vunit_kb*T);

```

```

01464     *U = pot*scale;
01465     *d2U = 0.0;
01466     dU[0] = -fx*scale;
01467     dU[1] = -fy*scale;
01468     dU[2] = -fz*scale;
01469
01470 #if 0
01471     /* Compare with old results */
01472     val = 0.0;
01473     Uold = 0.0; dUold[0] = 0.0; dUold[1] = 0.0; dUold[2] = 0.0;
01474     for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
01475         atom = Valist_getAtom(alist, iatom);
01476         position = Vatom_getPosition(atom);
01477         charge = Vatom_getCharge(atom);
01478         dist2 = 0;
01479         for (i=0; i<d; i++) {
01480             vec[i] = (position[i] - pt[i]);
01481             dist2 += VSQR(vec[i]);
01482         }
01483         dist = VSQRT(dist2);
01484
01485         /* POTENTIAL */
01486         Uold = Uold + charge/dist;
01487
01488         /* GRADIENT */
01489         for (i=0; i<d; i++) dUold[i] = dUold[i] + vec[i]*charge/(dist2*dist);
01490     }
01491     Uold = Uold*VSQR(Vunit_ec)*(1.0e10)/(4*VPI*Vunit_eps0*eps*Vunit_kb*T);
01492     for (i=0; i<d; i++) {
01493         dUold[i] = dUold[i]*VSQR(Vunit_ec)*(1.0e10)/(4*VPI*Vunit_eps0*eps*Vunit_kb*T);
01494     }
01495
01496     printf("Unew - Uold = %g - %g = %g\n", *U, Uold, (*U - Uold));
01497     printf("||dUnew - dUold||^2 = %g\n", (VSQR(dU[0] - dUold[0])
01498         + VSQR(dU[1] - dUold[1]) + VSQR(dU[2] - dUold[2])));
01499     printf("dUnew[0] = %g, dUold[0] = %g\n", dU[0], dUold[0]);
01500     printf("dUnew[1] = %g, dUold[1] = %g\n", dU[1], dUold[1]);
01501     printf("dUnew[2] = %g, dUold[2] = %g\n", dU[2], dUold[2]);
01502
01503 #endif
01504
01505 }
01506
01507
01508 VPUBLIC void Vfetk_PDE_initAssemble(PDE *thee, int ip[], double rp[]) {
01509
01510 #if 1
01511     /* Re-initialize the Green's function oracle in case the atom list has
01512      * changed */
01513     if (var.initGreen) {
01514         Vgreen_dtor(&(var.green));
01515         var.initGreen = 0;
01516     }
01517     var.green = Vgreen_ctor(var.fetk->pbe->alist);
01518     var.initGreen = 1;
01519 #else
01520     if (!var.initGreen) {
01521         var.green = Vgreen_ctor(var.fetk->pbe->alist);
01522         var.initGreen = 1;
01523     }
01524 #endif
01525
01526 }
01527
01528 VPUBLIC void Vfetk_PDE_initElement(PDE *thee, int elementType, int chart,
01529     double tvx[][3], void *data) {
01530
01531     int i, j;
01532     double epsp, epsw;
01533
01534     /* We assume that the simplex has been passed in as the void *data *
01535      * argument. Store it */
01536     VASSERT(data != NULL);
01537     var.simp = (SS *)data;
01538
01539     /* save the element type */
01540     var.sType = elementType;
01541
01542     /* Grab the vertices from this simplex */
01543     var.nverts = thee->dim+1;
01544     for (i=0; i<thee->dim+1; i++) var.verts[i] = SS_vertex(var.simp, i);

```

```

01545
01546     /* Vertex locations of this simplex */
01547     for (i=0; i<thee->dim+1; i++) {
01548         for (j=0; j<thee->dim; j++) {
01549             var.vx[i][j] = tvx[i][j];
01550         }
01551     }
01552
01553     /* Set the dielectric constant for this element for use in the jump term *
01554     * of the residual-based error estimator. The value is set to the average
01555     * * value of the vertices */
01556     var.jumpDiel = 0; /* NOT IMPLEMENTED YET! */
01557 }
01558
01559 VPUBLIC void Vfetk_PDE_initFace(PDE *thee, int faceType, int chart,
01560     double tnvect[]) {
01561
01562     int i;
01563
01564     /* unit normal vector of this face */
01565     for (i=0; i<thee->dim; i++) var.nvec[i] = tnvect[i];
01566
01567     /* save the face type */
01568     var.fType = faceType;
01569 }
01570
01571 VPUBLIC void Vfetk_PDE_initPoint(PDE *thee, int pointType, int chart,
01572     double txq[], double tU[], double tdU[][3]) {
01573
01574     int i, j, ichop;
01575     double u2, coef2, eps_p;
01576     Vhal_PBEType pdetype;
01577     Vpbe *pbe = VNULL;
01578
01579     eps_p = Vpbe_getSoluteDiel(var.fetk->pbe);
01580     pdetype = var.fetk->type;
01581     pbe = var.fetk->pbe;
01582
01583     /* the point, the solution value and gradient, and the Coulomb value and *
01584     * gradient at the point */
01585     if ((pdetype == PBE_LRPBE) || (pdetype == PBE_NRPBE)) {
01586         coulomb(pbe, thee->dim, txq, eps_p, &(var.W), var.dW, &(var.d2W));
01587     }
01588     for (i=0; i<thee->vec; i++) {
01589         var.U[i] = tU[i];
01590         for (j=0; j<thee->dim; j++) {
01591             var.xq[j] = txq[j];
01592             var.dU[i][j] = tdU[i][j];
01593         }
01594     }
01595
01596     /* interior form case */
01597     if (pointType == 0) {
01598
01599         /* Get the dielectric values */
01600         var.diel = diel();
01601         var.ionacc = ionacc();
01602         var.A = var.diel;
01603         var.F = (var.diel - eps_p);
01604
01605         switch (pdetype) {
01606
01607             case PBE_LPBE:
01608                 var.DB = var.ionacc*var.zkappa2*var.ionstr;
01609                 var.B = var.DB*var.U[0];
01610                 break;
01611
01612             case PBE_NPBE:
01613
01614                 var.B = 0;
01615                 var.DB = 0;
01616                 if ((var.ionacc > VSMALL) && (var.zks2 > VSMALL)) {
01617                     for (i=0; i<var.nion; i++) {
01618                         u2 = -1.0 * var.U[0] * var.ionQ[i];
01619
01620                         /* NONLINEAR TERM */
01621                         coef2 = -1.0 * var.ionacc * var.zks2 * var.ionConc[i];
01622                         var.B += (coef2 * Vcap_exp(u2, &ichop));
01623                         /* LINEARIZED TERM */
01624                         coef2 = -1.0 * var.ionQ[i] * coef2;
01625                         var.DB += (coef2 * Vcap_exp(u2, &ichop));

```

```

01626         }
01627     }
01628     break;
01629
01630     case PBE_LRPBE:
01631         var.DB = var.ionacc*var.zkappa2*var.ionstr;
01632         var.B = var.DB*(var.U[0]+var.W);
01633         break;
01634
01635     case PBE_NRPBE:
01636
01637         var.B = 0;
01638         var.DB = 0;
01639         if ((var.ionacc > VSMALL) && (var.zks2 > VSMALL)) {
01640             for (i=0; i<var.nion; i++) {
01641                 u2 = -1.0 * (var.U[0] + var.W) * var.ionQ[i];
01642
01643                 /* NONLINEAR TERM */
01644                 coef2 = -1.0 * var.ionacc * var.zks2 * var.ionConc[i];
01645                 var.B += (coef2 * Vcap_exp(u2, &ichop));
01646
01647                 /* LINEARIZED TERM */
01648                 coef2 = -1.0 * var.ionQ[i] * coef2;
01649                 var.DB += (coef2 * Vcap_exp(u2, &ichop));
01650             }
01651         }
01652         break;
01653
01654     case PBE_SMPBE: /* SMPBE Temp */
01655
01656         var.B = 0;
01657         var.DB = 0;
01658         if ((var.ionacc > VSMALL) && (var.zks2 > VSMALL)) {
01659             for (i=0; i<var.nion; i++) {
01660                 u2 = -1.0 * var.U[0] * var.ionQ[i];
01661
01662                 /* NONLINEAR TERM */
01663                 coef2 = -1.0 * var.ionacc * var.zks2 * var.ionConc[i];
01664                 var.B += (coef2 * Vcap_exp(u2, &ichop));
01665                 /* LINEARIZED TERM */
01666                 coef2 = -1.0 * var.ionQ[i] * coef2;
01667                 var.DB += (coef2 * Vcap_exp(u2, &ichop));
01668             }
01669         }
01670         break;
01671     default:
01672         Vnm_print(2, "Vfetk_PDE_initPoint: Unknown PBE type (%d)!\n",
01673                 pdetype);
01674         VASSERT(0);
01675         break;
01676 }
01677
01678 /* boundary form case */
01679 } else {
01680 #ifdef DONEUMANN
01681     ;
01682 #else
01683     Vnm_print(2, "Vfetk: Whoa! I just got a boundary point to evaluate (%d)!\n", pointType);
01684     Vnm_print(2, "Vfetk: Did you do that on purpose?\n");
01685 #endif
01686 }
01687
01688 #if 0 /* THIS IS VERY NOISY! */
01689     Vfetk_dumpLocalVar();
01690 #endif
01691
01692 }
01693
01694
01695 VPUBLIC void Vfetk_PDE_Fu(PDE *thee, int key, double F[]) {
01696
01697     //Vnm_print(2, "Vfetk_PDE_Fu: Setting error to zero!\n");
01698
01699     F[0] = 0.;
01700
01701 }
01702
01703 VPUBLIC double Vfetk_PDE_Fu_v(
01704     PDE *thee,
01705     int key,
01706     double V[],

```

```

01707         double dV[][VAPBS_DIM]
01708     ) {
01709
01710     Vhal_PBEType type;
01711     int i;
01712     double value = 0.;
01713
01714     type = var.fetk->type;
01715
01716     /* interior form case */
01717     if (key == 0) {
01718
01719         for (i=0; i<thee->dim; i++) value += ( var.A * var.dU[0][i] * dV[0][i] );
01720         value += var.B * V[0];
01721
01722         if ((type == PBE_LRPBE) || (type == PBE_NRPBE)) {
01723             for (i=0; i<thee->dim; i++) {
01724                 if (var.F > VSMALL) value += (var.F * var.dW[i] * dV[0][i]);
01725             }
01726         }
01727
01728     /* boundary form case */
01729     } else {
01730 #ifdef DONEUMANN
01731         value = 0.0;
01732 #else
01733         Vnm_print(2, "Vfetk: Whoa! I was just asked to evaluate a boundary weak form for point type
01734 %d!\n", key);
01735 #endif
01736     }
01737     var.Fu_v = value;
01738     return value;
01739 }
01740
01741 VPUBLIC double Vfetk_PDE_DFu_wv(
01742     PDE *thee,
01743     int key,
01744     double W[],
01745     double dW[][VAPBS_DIM],
01746     double V[],
01747     double dV[][3]
01748 ) {
01749
01750     Vhal_PBEType type;
01751     int i;
01752     double value = 0.;
01753
01754     type = var.fetk->type;
01755
01756     /* Interior form */
01757     if (key == 0) {
01758         value += var.DB * W[0] * V[0];
01759         for (i=0; i<thee->dim; i++) value += ( var.A * dW[0][i] * dV[0][i] );
01760
01761     /* boundary form case */
01762     } else {
01763 #ifdef DONEUMANN
01764         value = 0.0;
01765 #else
01766         Vnm_print(2, "Vfetk: Whoa! I was just asked to evaluate a boundary weak form for point type
01767 %d!\n", key);
01768 #endif
01769     }
01770     var.DFu_wv = value;
01771     return value;
01772 }
01773
01776 #define VRINGMAX 1000
01779 #define VATOMMAX 1000000
01780 VPUBLIC void Vfetk_PDE_delta(PDE *thee, int type, int chart, double txq[],
01781     void *user, double F[]) {
01782
01783     int iatom, jatom, natoms, atomIndex, atomList[VATOMMAX], nAtomList;
01784     int gotAtom, numSring, isimp, invert, sid;
01785     double *position, charge, phi[VAPBS_NVS], phix[VAPBS_NVS][3], value;
01786     Vatom *atom;
01787     Vhal_PBEType pdetype;
01788     SS *sring[VRINGMAX];
01789     VV *vertex = (VV *)user;

```

```

01790
01791     pdetype = var.fetk->type;
01792
01793     F[0] = 0.0;
01794
01795     if ((pdetype == PBE_LPBE) || (pdetype == PBE_NPBE) || (pdetype == PBE_SMPBE) /* SMPBE Added */) {
01796         VASSERT( vertex != VNULL);
01797         numSring = 0;
01798         sring[numSring] = VV_firstSS(vertex);
01799         while (sring[numSring] != VNULL) {
01800             numSring++;
01801             sring[numSring] = SS_link(sring[numSring-1], vertex);
01802         }
01803         VASSERT( numSring > 0 );
01804         VASSERT( numSring <= VRINGMAX );
01805
01806         /* Move around the simplex ring and determine the charge locations */
01807         F[0] = 0.;
01808         charge = 0.;
01809         nAtomList = 0;
01810         for (isimp=0; isimp<numSring; isimp++) {
01811             sid = SS_id(sring[isimp]);
01812             natoms = Vcsm_getNumberAtoms(Vfetk_getVcsm(var.fetk), sid);
01813             for (iatom=0; iatom<natoms; iatom++) {
01814                 /* Get the delta function information */
01815                 atomIndex = Vcsm_getAtomIndex(Vfetk_getVcsm(var.fetk),
01816                     iatom, sid);
01817                 gotAtom = 0;
01818                 for (jatom=0; jatom<nAtomList; jatom++) {
01819                     if (atomList[jatom] == atomIndex) {
01820                         gotAtom = 1;
01821                         break;
01822                     }
01823                 }
01824                 if (!gotAtom) {
01825                     VASSERT(nAtomList < VATOMMAX);
01826                     atomList[nAtomList] = atomIndex;
01827                     nAtomList++;
01828
01829                     atom = Vcsm_getAtom(Vfetk_getVcsm(var.fetk), iatom, sid);
01830                     charge = Vatom_getCharge(atom);
01831                     position = Vatom_getPosition(atom);
01832
01833                     /* Get the test function value at the delta function I
01834                      * used to do a VASSERT to make sure the point was in the
01835                      * simplex (i.e., make sure round-off error isn't an
01836                      * issue), but round off errors became an issue */
01837                     if (!Gem_pointInSimplexVal(Vfetk_getGem(var.fetk),
01838                         sring[isimp], position, phi, phix)) {
01839                         if (!Gem_pointInSimplex(Vfetk_getGem(var.fetk),
01840                             sring[isimp], position)) {
01841                             Vnm_print(2, "delta: Both Gem_pointInSimplexVal \
01842 and Gem_pointInSimplex detected misplaced point charge!\n");
01843                             Vnm_print(2, "delta: I think you have problems: \
01844 phi = {}");
01845                             for (ivert=0; ivert<Gem_dimVV(Vfetk_getGem(var.fetk)); ivert++) Vnm_print(2,
01846                                 "%e ", phi[ivert]);
01847                             Vnm_print(2, "}\n");
01848                         }
01849                         value = 0;
01850                         for (ivert=0; ivert<Gem_dimVV(Vfetk_getGem(var.fetk)); ivert++) {
01851                             if (VV_id(SS_vertex(sring[isimp], ivert)) == VV_id(vertex)) value += phi[ivert];
01852                         }
01853
01854                         F[0] += (value * Vpbe_getZmagic(var.fetk->pbe) * charge);
01855                     } /* if !gotAtom */
01856                 } /* for iatom */
01857             } /* for isimp */
01858
01859         } else if ((pdetype == PBE_LRPBE) || (pdetype == PBE_NRPBE)) {
01860             F[0] = 0.0;
01861         } else { VASSERT(0); }
01862
01863         var.delta = F[0];
01864     }
01865 }
01866
01867 VPUBLIC void Vfetk_PDE_u_D(PDE *thee, int type, int chart, double txq[],
01868     double F[]) {

```



```

01869
01870     if ((var.fetk->type == PBE_LPBE) || (var.fetk->type == PBE_NPBE) || (var.fetk->type == PBE_SMPBE) /*
SMPBE Added */) {
01871         F[0] = debye_U(var.fetk->pbe, thee->dim, txq);
01872     } else if ((var.fetk->type == PBE_LRPBE) || (var.fetk->type == PBE_NRPBE)) {
01873         F[0] = debye_Udiff(var.fetk->pbe, thee->dim, txq);
01874     } else VASSERT(0);
01875
01876     var.u_D = F[0];
01877
01878 }
01879
01886 VPUBLIC void Vfetk_PDE_u_T(PDE *thee, int type, int chart, double txq[],
01887     double F[]) {
01888     /*VPUBLIC void Vfetk_PDE_u_T(sPDE *thee,
01889         int type,
01890         int chart,
01891         double txq[],
01892         double F[],
01893         double dF[][3]
01894     ) { */
01895
01896     F[0] = 0.0;
01897     var.u_T = F[0];
01898
01899 }
01900
01901
01902 VPUBLIC void Vfetk_PDE_bisectEdge(int dim, int dimII, int edgeType,
01903     int chart[], double vx[][3]) {
01904
01905     int i;
01906
01907     for (i=0; i<dimII; i++) vx[2][i] = .5 * (vx[0][i] + vx[1][i]);
01908     chart[2] = chart[0];
01909
01910 }
01911
01912 VPUBLIC void Vfetk_PDE_mapBoundary(int dim, int dimII, int vertexType,
01913     int chart, double vx[3]) {
01914
01915 }
01916
01917 VPUBLIC int Vfetk_PDE_markSimplex(int dim, int dimII, int simplexType,
01918     int faceType[VAPBS_NVS], int vertexType[VAPBS_NVS], int chart[], double vx[][3],
01919     void *simplex) {
01920
01921     double targetRes, edgeLength, srad, swin, myAcc, refAcc;
01922     int i, natoms;
01923     Vsurf_Meth srfm;
01924     Vhal_PBEType type;
01925     FEMparm *feparm = VNULL;
01926     PBEparm *pbeparm = VNULL;
01927     Vpbe *pbe = VNULL;
01928     Vacc *acc = VNULL;
01929     Vcsm *csm = VNULL;
01930     SS *simp = VNULL;
01931
01932     VASSERT(var.fetk->feparm != VNULL);
01933     feparm = var.fetk->feparm;
01934     VASSERT(var.fetk->pbeparm != VNULL);
01935     pbeparm = var.fetk->pbeparm;
01936     pbe = var.fetk->pbe;
01937     csm = Vfetk_getVcsm(var.fetk);
01938     acc = pbe->acc;
01939     targetRes = feparm->targetRes;
01940     srfm = pbeparm->srfm;
01941     srad = pbeparm->srad;
01942     swin = pbeparm->swin;
01943     simp = (SS *)simplex;
01944     type = var.fetk->type;
01945
01946     /* Check to see if this simplex is smaller than the target size */
01947     /* NAB WARNING: I am providing face=-1 here to conform to the new MC API; however, I'm not sure if
this is the correct behavior. */
01948     Gem_longestEdge(var.fetk->gm, simp, -1, &edgeLength);
01949     if (edgeLength < targetRes) return 0;
01950
01951     /* For non-regularized PBE, check charge-simplex map */
01952     if ((type == PBE_LPBE) || (type == PBE_NPBE) || (type == PBE_SMPBE) /* SMPBE Added */) {
01953         natoms = Vcsm_getNumberAtoms(csm, SS_id(simp));

```

```

01954         if (natoms > 0) {
01955             return 1;
01956         }
01957     }
01958
01959     /* We would like to resolve the mesh between the van der Waals surface the
01960     * max distance from this surface where there could be coefficient
01961     * changes */
01962     switch(srfm) {
01963     case VSM_MOL:
01964         refAcc = Vacc_molAcc(acc, vx[0], srad);
01965         for (i=1; i<(dim+1); i++) {
01966             myAcc = Vacc_molAcc(acc, vx[i], srad);
01967             if (myAcc != refAcc) {
01968                 return 1;
01969             }
01970         }
01971         break;
01972     case VSM_MOLSMOOTH:
01973         refAcc = Vacc_molAcc(acc, vx[0], srad);
01974         for (i=1; i<(dim+1); i++) {
01975             myAcc = Vacc_molAcc(acc, vx[i], srad);
01976             if (myAcc != refAcc) {
01977                 return 1;
01978             }
01979         }
01980         break;
01981     case VSM_SPLINE:
01982         refAcc = Vacc_splineAcc(acc, vx[0], swin, 0.0);
01983         for (i=1; i<(dim+1); i++) {
01984             myAcc = Vacc_splineAcc(acc, vx[i], swin, 0.0);
01985             if (myAcc != refAcc) {
01986                 return 1;
01987             }
01988         }
01989         break;
01990     default:
01991         VASSERT(0);
01992         break;
01993     }
01994
01995     return 0;
01996 }
01997
01998 VPUBLIC void Vfetc_PDE_oneChart(int dim, int dimII, int objType, int chart[],
01999     double vx[][3], int dimV) {
02000
02001 }
02002
02003 VPUBLIC double Vfetc_PDE_Ju(PDE *thee, int key) {
02004
02005     int i, ichop;
02006     double dielE, qmE, coef2, u2;
02007     double value = 0.;
02008     Vhal_PBEType type;
02009
02010     type = var.fetc->type;
02011
02012     /* interior form case */
02013     if (key == 0) {
02014         dielE = 0;
02015         for (i=0; i<3; i++) dielE += VSQR(var.dU[0][i]);
02016         dielE = dielE*var.diel;
02017
02018         switch (type) {
02019         case PBE_LPBE:
02020             if ((var.ionacc > VSMALL) && (var.zkappa2 > VSMALL)) {
02021                 qmE = var.ionacc*var.zkappa2*VSQR(var.U[0]);
02022             } else qmE = 0;
02023             break;
02024         case PBE_NPBE:
02025             if ((var.ionacc > VSMALL) && (var.zks2 > VSMALL)) {
02026                 qmE = 0.;
02027                 for (i=0; i<var.nion; i++) {
02028                     coef2 = var.ionacc * var.zks2 * var.ionConc[i] * var.ionQ[i];
02029                     u2 = -1.0 * (var.U[0]) * var.ionQ[i];
02030                     qmE += (coef2 * (Vcap_exp(u2, &ichop) - 1.0));
02031                 }
02032             } else qmE = 0;
02033             break;
02034         case PBE_LRPBE:

```

```

02035         if ((var.ionacc > VSMALL) && (var.zkappa2 > VSMALL)) {
02036             qmE = var.ionacc*var.zkappa2*VSQR((var.U[0] + var.W));
02037         } else qmE = 0;
02038         break;
02039     case PBE_NRPBE:
02040         if ((var.ionacc > VSMALL) && (var.zks2 > VSMALL)) {
02041             qmE = 0.;
02042             for (i=0; i<var.nion; i++) {
02043                 coef2 = var.ionacc * var.zks2 * var.ionConc[i] * var.ionQ[i];
02044                 u2 = -1.0 * (var.U[0] + var.W) * var.ionQ[i];
02045                 qmE += (coef2 * (Vcap_exp(u2, &ichop) - 1.0));
02046             }
02047         } else qmE = 0;
02048         break;
02049     case PBE_SMPBE: /* SMPBE Temp */
02050         if ((var.ionacc > VSMALL) && (var.zks2 > VSMALL)) {
02051             qmE = 0.;
02052             for (i=0; i<var.nion; i++) {
02053                 coef2 = var.ionacc * var.zks2 * var.ionConc[i] * var.ionQ[i];
02054                 u2 = -1.0 * (var.U[0]) * var.ionQ[i];
02055                 qmE += (coef2 * (Vcap_exp(u2, &ichop) - 1.0));
02056             }
02057         } else qmE = 0;
02058         break;
02059     default:
02060         Vnm_print(2, "Vfetk_PDE_Ju: Invalid PBE type (%d)!\n", type);
02061         VASSERT(0);
02062         break;
02063     }
02064
02065     value = 0.5*(dielE + qmE)/Vpbe_getZmagic(var.fetk->pbe);
02066
02067     /* boundary form case */
02068     } else if (key == 1) {
02069         value = 0.0;
02070
02071         /* how did we get here? */
02072     } else VASSERT(0);
02073
02074     return value;
02075 }
02076 }
02077
02078 VPUBLIC void Vfetk_externalUpdateFunction(SS **sims, int num) {
02079     Vcsm *csm = VNULL;
02080     int rc;
02081
02082     VASSERT(var.fetk != VNULL);
02083     csm = Vfetk_getVcsm(var.fetk);
02084     VASSERT(csm != VNULL);
02085
02086     rc = Vcsm_update(csm, sims, num);
02087
02088     if (!rc) {
02089         Vnm_print(2, "Error while updating charge-simplex map!\n");
02090         VASSERT(0);
02091     }
02092 }
02093 }
02094
02095 VPRIVATE void polyEval(int numP, double p[], double c[][VMAXP], double xv[]) {
02096     int i;
02097     double x, y, z;
02098
02099     x = xv[0];
02100     y = xv[1];
02101     z = xv[2];
02102     for (i=0; i<numP; i++) {
02103         p[i] = c[i][0]
02104             + c[i][1] * x
02105             + c[i][2] * y
02106             + c[i][3] * z
02107             + c[i][4] * x*x
02108             + c[i][5] * y*y
02109             + c[i][6] * z*z
02110             + c[i][7] * x*y
02111             + c[i][8] * x*z
02112             + c[i][9] * y*z
02113             + c[i][10] * x*x*x
02114             + c[i][11] * y*y*y
02115             + c[i][12] * z*z*z

```

```

02116         + c[i][13] * x*x*y
02117         + c[i][14] * x*x*z
02118         + c[i][15] * x*y*y
02119         + c[i][16] * y*y*z
02120         + c[i][17] * x*z*z
02121         + c[i][18] * y*z*z;
02122     }
02123 }
02124
02125 VPRIVATE void setCoef(int numP, double c[][VMAXP], double cx[][VMAXP],
02126     double cy[][VMAXP], double cz[][VMAXP], int ic[][VMAXP], int icx[][VMAXP],
02127     int icy[][VMAXP], int icz[][VMAXP]) {
02128     int i, j;
02129     for (i=0; i<numP; i++) {
02130         for (j=0; j<VMAXP; j++) {
02131             c[i][j] = 0.5 * (double)ic[i][j];
02132             cx[i][j] = 0.5 * (double)icx[i][j];
02133             cy[i][j] = 0.5 * (double)icy[i][j];
02134             cz[i][j] = 0.5 * (double)icz[i][j];
02135         }
02136     }
02137 }
02138 }
02139
02140 VPUBLIC int Vfetk_PDE_simplexBasisInit(int key, int dim, int comp, int *ndof,
02141     int dof[]) {
02142     int qorder, bump, dimIS[VAPBS_NVS];
02143
02144     /* necessary quadrature order to return at the end */
02145     qorder = P_DEG;
02146
02147     /* deal with bump function requests */
02148     if ((key == 0) || (key == 1)) {
02149         bump = 0;
02150     } else if ((key == 2) || (key == 3)) {
02151         bump = 1;
02152     } else { VASSERT(0); }
02153
02154     /* for now use same element for all components, both trial and test */
02155     if (dim==2) {
02156         /* 2D simplex dimensions */
02157         dimIS[0] = 3; /* number of vertices */
02158         dimIS[1] = 3; /* number of edges */
02159         dimIS[2] = 0; /* number of faces (3D only) */
02160         dimIS[3] = 1; /* number of simplices (always=1) */
02161         if (bump==0) {
02162             if (P_DEG==1) {
02163                 init_2DPl(dimIS, ndof, dof, c, cx, cy, cz);
02164             } else if (P_DEG==2) {
02165                 init_2DPl(dimIS, ndof, dof, c, cx, cy, cz);
02166             } else if (P_DEG==3) {
02167                 init_2DPl(dimIS, ndof, dof, c, cx, cy, cz);
02168             } else Vnm_print(2, "..bad order..");
02169         } else if (bump==1) {
02170             if (P_DEG==1) {
02171                 init_2DPl(dimIS, ndof, dof, c, cx, cy, cz);
02172             } else Vnm_print(2, "..bad order..");
02173         } else Vnm_print(2, "..bad bump..");
02174     } else if (dim==3) {
02175         /* 3D simplex dimensions */
02176         dimIS[0] = 4; /* number of vertices */
02177         dimIS[1] = 6; /* number of edges */
02178         dimIS[2] = 4; /* number of faces (3D only) */
02179         dimIS[3] = 1; /* number of simplices (always=1) */
02180         if (bump==0) {
02181             if (P_DEG==1) {
02182                 init_3DPl(dimIS, ndof, dof, c, cx, cy, cz);
02183             } else if (P_DEG==2) {
02184                 init_3DPl(dimIS, ndof, dof, c, cx, cy, cz);
02185             } else if (P_DEG==3) {
02186                 init_3DPl(dimIS, ndof, dof, c, cx, cy, cz);
02187             } else Vnm_print(2, "..bad order..");
02188         } else if (bump==1) {
02189             if (P_DEG==1) {
02190                 init_3DPl(dimIS, ndof, dof, c, cx, cy, cz);
02191             } else Vnm_print(2, "..bad order..");
02192         } else Vnm_print(2, "..bad bump..");
02193     } else Vnm_print(2, "..bad dimension..");
02194 }
02195
02196 /* save number of DF */

```

```

02197     numP = *ndof;
02198
02199     /* return the required quadrature order */
02200     return qorder;
02201 }
02202
02203 VPUBLIC void Vfetk_PDE_simplexBasisForm(int key, int dim, int comp, int pdkey,
02204     double xq[], double basis[]) {
02205
02206     if (pdkey == 0) {
02207         polyEval(numP, basis, c, xq);
02208     } else if (pdkey == 1) {
02209         polyEval(numP, basis, cx, xq);
02210     } else if (pdkey == 2) {
02211         polyEval(numP, basis, cy, xq);
02212     } else if (pdkey == 3) {
02213         polyEval(numP, basis, cz, xq);
02214     } else { VASSERT(0); }
02215 }
02216
02217 PRIVATE void init_2DP1(int dimIS[], int *ndof, int dof[], double c[][VMAXP],
02218     double cx[][VMAXP], double cy[][VMAXP], double cz[][VMAXP]) {
02219
02220     int i;
02221
02222     /* dof number and locations */
02223     dof[0] = 1;
02224     dof[1] = 0;
02225     dof[2] = 0;
02226     dof[3] = 0;
02227     *ndof = 0;
02228     for (i=0; i<VAPBS_NVS; i++) *ndof += dimIS[i] * dof[i];
02229     VASSERT( *ndof == dim_2DP1 );
02230     VASSERT( *ndof <= VMAXP );
02231
02232     /* coefficients of the polynomials */
02233     setCoef( *ndof, c, cx, cy, cz, lgr_2DP1, lgr_2DP1x, lgr_2DP1y, lgr_2DP1z );
02234 }
02235
02236 PRIVATE void init_3DP1(int dimIS[], int *ndof, int dof[], double c[][VMAXP],
02237     double cx[][VMAXP], double cy[][VMAXP], double cz[][VMAXP]) {
02238
02239     int i;
02240
02241     /* dof number and locations */
02242     dof[0] = 1;
02243     dof[1] = 0;
02244     dof[2] = 0;
02245     dof[3] = 0;
02246     *ndof = 0;
02247     for (i=0; i<VAPBS_NVS; i++) *ndof += dimIS[i] * dof[i];
02248     VASSERT( *ndof == dim_3DP1 );
02249     VASSERT( *ndof <= VMAXP );
02250
02251     /* coefficients of the polynomials */
02252     setCoef( *ndof, c, cx, cy, cz, lgr_3DP1, lgr_3DP1x, lgr_3DP1y, lgr_3DP1z );
02253 }
02254
02255 VPUBLIC void Vfetk_dumpLocalVar() {
02256
02257     int i;
02258
02259     Vnm_print(1, "DEBUG: nvec = (%g, %g, %g)\n", var.nvec[0], var.nvec[1],
02260         var.nvec[2]);
02261     Vnm_print(1, "DEBUG: nverts = %d\n", var.nverts);
02262     for (i=0; i<var.nverts; i++) {
02263         Vnm_print(1, "DEBUG: verts[%d] ID = %d\n", i, VV_id(var.verts[i]));
02264         Vnm_print(1, "DEBUG: vx[%d] = (%g, %g, %g)\n", i, var.vx[i][0],
02265             var.vx[i][1], var.vx[i][2]);
02266     }
02267     Vnm_print(1, "DEBUG: simp ID = %d\n", SS_id(var.simp));
02268     Vnm_print(1, "DEBUG: sType = %d\n", var.sType);
02269     Vnm_print(1, "DEBUG: fType = %d\n", var.fType);
02270     Vnm_print(1, "DEBUG: xq = (%g, %g, %g)\n", var.xq[0], var.xq[1], var.xq[2]);
02271     Vnm_print(1, "DEBUG: U[0] = %g\n", var.U[0]);
02272     Vnm_print(1, "DEBUG: dU[0] = (%g, %g, %g)\n", var.dU[0][0], var.dU[0][1],
02273         var.dU[0][2]);
02274     Vnm_print(1, "DEBUG: W = %g\n", var.W);
02275     Vnm_print(1, "DEBUG: d2W = %g\n", var.d2W);
02276     Vnm_print(1, "DEBUG: dW = (%g, %g, %g)\n", var.dW[0], var.dW[1], var.dW[2]);
02277     Vnm_print(1, "DEBUG: diel = %g\n", var.diel);

```

```

02278     Vnm_print(1, "DEBUG: ionacc = %g\n", var.ionacc);
02279     Vnm_print(1, "DEBUG: A = %g\n", var.A);
02280     Vnm_print(1, "DEBUG: F = %g\n", var.F);
02281     Vnm_print(1, "DEBUG: B = %g\n", var.B);
02282     Vnm_print(1, "DEBUG: DB = %g\n", var.DB);
02283     Vnm_print(1, "DEBUG: nion = %d\n", var.nion);
02284     for (i=0; i<var.nion; i++) {
02285         Vnm_print(1, "DEBUG: ionConc[%d] = %g\n", i, var.ionConc[i]);
02286         Vnm_print(1, "DEBUG: ionQ[%d] = %g\n", i, var.ionQ[i]);
02287         Vnm_print(1, "DEBUG: ionRadii[%d] = %g\n", i, var.ionRadii[i]);
02288     }
02289     Vnm_print(1, "DEBUG: zkappa2 = %g\n", var.zkappa2);
02290     Vnm_print(1, "DEBUG: zks2 = %g\n", var.zks2);
02291     Vnm_print(1, "DEBUG: Fu_v = %g\n", var.Fu_v);
02292     Vnm_print(1, "DEBUG: DFu_wv = %g\n", var.DFu_wv);
02293     Vnm_print(1, "DEBUG: delta = %g\n", var.delta);
02294     Vnm_print(1, "DEBUG: u_D = %g\n", var.u_D);
02295     Vnm_print(1, "DEBUG: u_T = %g\n", var.u_T);
02296
02297 };
02298
02299 VPUBLIC int Vfetk_fillArray(Vfetk *thee, Bvec *vec, Vdata_Type type) {
02300
02301     int i, j, ichop;
02302     double coord[3], chi, q, conc, val;
02303     VV *vert;
02304     Bvec *u, *u_d;
02305     AM *am;
02306     Gem *gm;
02307     PBEParm *pbeparm;
02308     Vacc *acc;
02309     Vpbe *pbe;
02310
02311     gm = thee->gm;
02312     am = thee->am;
02313     pbe = thee->pbe;
02314     pbeparm = thee->pbeparm;
02315     acc = pbe->acc;
02316
02317     /* Make sure vec has enough rows to accomodate the vertex data */
02318     if (Bvec_numRB(vec, 0) != Gem_numVV(gm)) {
02319         Vnm_print(2, "Vfetk_fillArray: insufficient space in Bvec!\n");
02320         Vnm_print(2, "Vfetk_fillArray: Have %d, need %d!\n", Bvec_numRB(vec, 0),
02321             Gem_numVV(gm));
02322         return 0;
02323     }
02324
02325     switch (type) {
02326
02327     case VDT_CHARGE:
02328         Vnm_print(2, "Vfetk_fillArray: can't write out charge distribution!\n");
02329         return 0;
02330         break;
02331
02332     case VDT_POT:
02333         u = am->u;
02334         u_d = am->ud;
02335         /* Copy in solution */
02336         Bvec_copy(vec, u);
02337         /* Add dirichlet condition */
02338         Bvec_axpy(vec, u_d, 1.0);
02339         break;
02340
02341     case VDT_SMOL:
02342         for (i=0; i<Gem_numVV(gm); i++) {
02343             vert = Gem_VV(gm, i);
02344             for (j=0; j<3; j++) coord[j] = VV_coord(vert, j);
02345             chi = Vacc_molAcc(acc, coord, pbe->solventRadius);
02346             Bvec_set(vec, i, chi);
02347         }
02348         break;
02349
02350     case VDT_SSPL:
02351         for (i=0; i<Gem_numVV(gm); i++) {
02352             vert = Gem_VV(gm, i);
02353             for (j=0; j<3; j++) coord[j] = VV_coord(vert, j);
02354             chi = Vacc_splineAcc(acc, coord, pbeparm->swin, 0.0);
02355             Bvec_set(vec, i, chi);
02356         }
02357         break;
02358

```

```

02359     case VDT_VDW:
02360         for (i=0; i<Gem_numVV(gm); i++) {
02361             vert = Gem_VV(gm, i);
02362             for (j=0; j<3; j++) coord[j] = VV_coord(vert, j);
02363             chi = Vacc_vdwAcc(acc, coord);
02364             Bvec_set(vec, i, chi);
02365         }
02366         break;
02367
02368     case VDT_IVDW:
02369         for (i=0; i<Gem_numVV(gm); i++) {
02370             vert = Gem_VV(gm, i);
02371             for (j=0; j<3; j++) coord[j] = VV_coord(vert, j);
02372             chi = Vacc_ivdwAcc(acc, coord, pbe->maxIonRadius);
02373             Bvec_set(vec, i, chi);
02374         }
02375         break;
02376
02377     case VDT_LAP:
02378         Vnm_print(2, "Vfetk_fillArray: can't write out Laplacian!\n");
02379         return 0;
02380         break;
02381
02382     case VDT_EDENS:
02383         Vnm_print(2, "Vfetk_fillArray: can't write out energy density!\n");
02384         return 0;
02385         break;
02386
02387     case VDT_NDENS:
02388         u = am->u;
02389         u_d = am->ud;
02390         /* Copy in solution */
02391         Bvec_copy(vec, u);
02392         /* Add dirichlet condition */
02393         Bvec_axpy(vec, u_d, 1.0);
02394         /* Load up ions */
02395         ichop = 0;
02396         for (i=0; i<Gem_numVV(gm); i++) {
02397             val = 0;
02398             for (j=0; j<pbe->numIon; j++) {
02399                 q = pbe->ionQ[j];
02400                 conc = pbe->ionConc[j];
02401                 if (thee->type == PBE_NPBE || thee->type == PBE_SMPBE /* SMPBE Added */) {
02402                     val += (conc*Vcap_exp(-q*Bvec_val(vec, i), &ichop));
02403                 } else if (thee->type == PBE_LPBE) {
02404                     val += (conc * (1 - q*Bvec_val(vec, i)));
02405                 }
02406             }
02407             Bvec_set(vec, i, val);
02408         }
02409         break;
02410
02411     case VDT_QDENS:
02412         u = am->u;
02413         u_d = am->ud;
02414         /* Copy in solution */
02415         Bvec_copy(vec, u);
02416         /* Add dirichlet condition */
02417         Bvec_axpy(vec, u_d, 1.0);
02418         /* Load up ions */
02419         ichop = 0;
02420         for (i=0; i<Gem_numVV(gm); i++) {
02421             val = 0;
02422             for (j=0; j<pbe->numIon; j++) {
02423                 q = pbe->ionQ[j];
02424                 conc = pbe->ionConc[j];
02425                 if (thee->type == PBE_NPBE || thee->type == PBE_SMPBE /* SMPBE Added */) {
02426                     val += (q*conc*Vcap_exp(-q*Bvec_val(vec, i), &ichop));
02427                 } else if (thee->type == PBE_LPBE) {
02428                     val += (q*conc*(1 - q*Bvec_val(vec, i)));
02429                 }
02430             }
02431             Bvec_set(vec, i, val);
02432         }
02433         break;
02434
02435     case VDT_DIELX:
02436         Vnm_print(2, "Vfetk_fillArray: can't write out x-shifted diel!\n");
02437         return 0;
02438         break;
02439

```

```

02440         case VDT_DIELY:
02441             Vnm_print(2, "Vfetc_fillArray: can't write out y-shifted diel!\n");
02442             return 0;
02443             break;
02444
02445         case VDT_DIELZ:
02446             Vnm_print(2, "Vfetc_fillArray: can't write out z-shifted diel!\n");
02447             return 0;
02448             break;
02449
02450         case VDT_KAPPA:
02451             Vnm_print(2, "Vfetc_fillArray: can't write out kappa!\n");
02452             return 0;
02453             break;
02454
02455         default:
02456             Vnm_print(2, "Vfetc_fillArray: invalid data type (%d)!\n", type);
02457             return 0;
02458             break;
02459     }
02460
02461     return 1;
02462 }
02463
02464 VPUBLIC int Vfetc_write(Vfetc *thee, const char *iodev, const char *iofmt,
02465     const char *thost, const char *fname, Bvec *vec, Vdata_Format format) {
02466
02467     int i, j, ichop;
02468     Aprx *aprx;
02469     Gem *gm;
02470     Vio *sock;
02471
02472     VASSERT(thee != VNULL);
02473     aprx = thee->aprx;
02474     gm = thee->gm;
02475
02476     sock = Vio_ctor(iodev, iofmt, thost, fname, "w");
02477     if (sock == VNULL) {
02478         Vnm_print(2, "Vfetc_write: Problem opening virtual socket %s\n",
02479             fname);
02480         return 0;
02481     }
02482     if (Vio_connect(sock, 0) < 0) {
02483         Vnm_print(2, "Vfetc_write: Problem connecting to virtual socket %s\n",
02484             fname);
02485         return 0;
02486     }
02487
02488     /* Make sure vec has enough rows to accomodate the vertex data */
02489     if (Bvec_numRB(vec, 0) != Gem_numVV(gm)) {
02490         Vnm_print(2, "Vfetc_fillArray: insufficient space in Bvec!\n");
02491         Vnm_print(2, "Vfetc_fillArray: Have %d, need %d!\n", Bvec_numRB(vec, 0),
02492             Gem_numVV(gm));
02493         return 0;
02494     }
02495
02496     switch (format) {
02497
02498         case VDF_DX:
02499             Aprx_writeSQL(aprx, sock, vec, "DX");
02500             break;
02501
02502         case VDF_AVS:
02503             Aprx_writeSQL(aprx, sock, vec, "UCD");
02504             break;
02505
02506         case VDF_UHBD:
02507             Vnm_print(2, "Vfetc_write: UHBD format not supported!\n");
02508             return 0;
02509
02510         default:
02511             Vnm_print(2, "Vfetc_write: Invalid data format (%d)!\n", format);
02512             return 0;
02513     }
02514
02515     Vio_connectFree(sock);
02516     Vio_dtor(&sock);
02517
02518     return 1;
02519 }

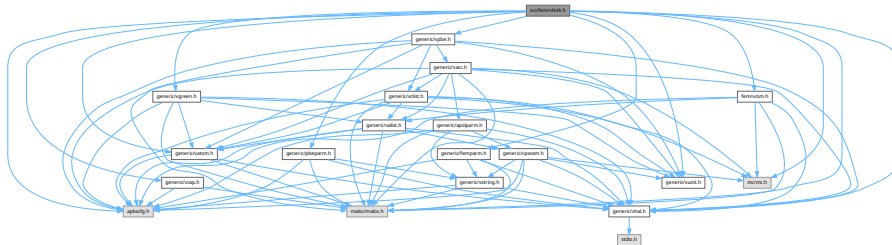
```


9.10 src/fem/vfetk.h File Reference

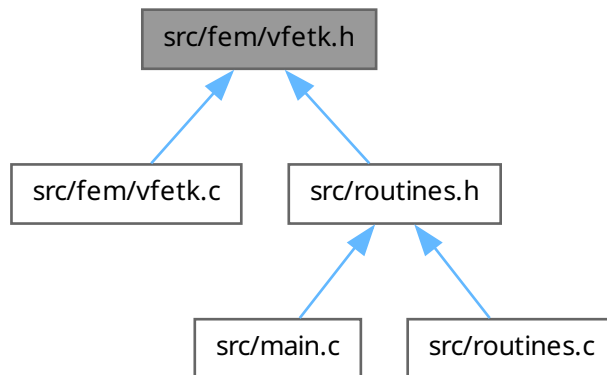
Contains declarations for class Vfetk.

```
#include "apbscfg.h"
#include "maloc/maloc.h"
#include "mc/mc.h"
#include "generic/vhal.h"
#include "generic/vatom.h"
#include "generic/vpbe.h"
#include "generic/vunit.h"
#include "generic/vgreen.h"
#include "generic/vcap.h"
#include "generic/pbeparm.h"
#include "generic/femparm.h"
#include "fem/vcsm.h"
```

Include dependency graph for vfetk.h:



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [sVfetk](#)

Contains public data members for Vfetk class/module.

- struct [sVfetk_LocalVar](#)
Vfetk LocalVar subclass.

Typedefs

- typedef enum [eVfetk_LsolvType](#) [Vfetk_LsolvType](#)
Declare FEMparm_LsolvType type.
- typedef enum [eVfetk_MeshLoad](#) [Vfetk_MeshLoad](#)
Declare FEMparm_GuessType type.
- typedef enum [eVfetk_NsolvType](#) [Vfetk_NsolvType](#)
Declare FEMparm_NsolvType type.
- typedef enum [eVfetk_GuessType](#) [Vfetk_GuessType](#)
Declare FEMparm_GuessType type.
- typedef enum [eVfetk_PrecType](#) [Vfetk_PrecType](#)
Declare FEMparm_GuessType type.
- typedef struct [sVfetk](#) [Vfetk](#)
- typedef struct [sVfetk_LocalVar](#) [Vfetk_LocalVar](#)
Declaration of the Vfetk_LocalVar subclass as the Vfetk_LocalVar structure.

Enumerations

- enum [eVfetk_LsolvType](#) { [VLT_SLU](#) =0 , [VLT_MG](#) =1 , [VLT_CG](#) =2 , [VLT_BCG](#) =3 }
Linear solver type.
- enum [eVfetk_MeshLoad](#) { [VML_DIRICUBE](#) , [VML_NEUMCUBE](#) , [VML_EXTERNAL](#) }
Mesh loading operation.
- enum [eVfetk_NsolvType](#) { [VNT_NEW](#) =0 , [VNT_INC](#) =1 , [VNT_ARC](#) =2 }
Non-linear solver type.
- enum [eVfetk_GuessType](#) { [VGT_ZERO](#) =0 , [VGT_DIRI](#) =1 , [VGT_PREV](#) =2 }
Initial guess type.
- enum [eVfetk_PrecType](#) { [VPT_IDEN](#) =0 , [VPT_DIAG](#) =1 , [VPT_MG](#) =2 }
Preconditioner type.

Functions

- VEXTERNC Gem * [Vfetk_getGem](#) ([Vfetk](#) *thee)
Get a pointer to the Gem (grid manager) object.
- VEXTERNC AM * [Vfetk_getAM](#) ([Vfetk](#) *thee)
Get a pointer to the AM (algebra manager) object.
- VEXTERNC [Vpbe](#) * [Vfetk_getVpbe](#) ([Vfetk](#) *thee)
Get a pointer to the Vpbe (PBE manager) object.
- VEXTERNC [Vcsm](#) * [Vfetk_getVcsm](#) ([Vfetk](#) *thee)
Get a pointer to the Vcsm (charge-simplex map) object.
- VEXTERNC int [Vfetk_getAtomColor](#) ([Vfetk](#) *thee, int iatom)
Get the partition information for a particular atom.
- VEXTERNC [Vfetk](#) * [Vfetk_ctor](#) ([Vpbe](#) *pbe, [Vhal_PBEType](#) type)
Constructor for Vfetk object.
- VEXTERNC int [Vfetk_ctor2](#) ([Vfetk](#) *thee, [Vpbe](#) *pbe, [Vhal_PBEType](#) type)
FORTTRAN stub constructor for Vfetk object.
- VEXTERNC void [Vfetk_dtor](#) ([Vfetk](#) **thee)

- Object destructor.*

 - VEXTERNC void [Vfetk_dtor2](#) ([Vfetk](#) *thee)
- FORTRAN stub object destructor.*

 - VEXTERNC double * [Vfetk_getSolution](#) ([Vfetk](#) *thee, int *length)

Create an array containing the solution (electrostatic potential in units of $k_B T/e$) at the finest mesh level.
- VEXTERNC void [Vfetk_setParameters](#) ([Vfetk](#) *thee, [PBEparm](#) *pbeparm, [FEMparm](#) *feparm)

Set the parameter objects.
- VPUBLIC double [Vfetk_energy](#) ([Vfetk](#) *thee, int color, int nonlin)

Return the total electrostatic energy.
- VEXTERNC double [Vfetk_dqmEnergy](#) ([Vfetk](#) *thee, int color)

Get the "mobile charge" and "polarization" contributions to the electrostatic energy.
- VEXTERNC double [Vfetk_qfEnergy](#) ([Vfetk](#) *thee, int color)

Get the "fixed charge" contribution to the electrostatic energy.
- VEXTERNC unsigned long int [Vfetk_memChk](#) ([Vfetk](#) *thee)

Return the memory used by this structure (and its contents) in bytes.
- VEXTERNC void [Vfetk_setAtomColors](#) ([Vfetk](#) *thee)

Transfer color (partition ID) information from a partitioned mesh to the atoms.
- VEXTERNC void [Bmat_printHB](#) ([Bmat](#) *thee, char *fname)

Writes a Bmat to disk in Harwell-Boeing sparse matrix format.
- VEXTERNC Vrc_Codes [Vfetk_genCube](#) ([Vfetk](#) *thee, double center[3], double length[3], [Vfetk_MeshLoad](#) meshType)

Construct a rectangular mesh (in the current Vfetk object)
- VEXTERNC Vrc_Codes [Vfetk_loadMesh](#) ([Vfetk](#) *thee, double center[3], double length[3], [Vfetk_MeshLoad](#) meshType, Vio *sock)

Loads a mesh into the Vfetk (and associated) object(s).
- VEXTERNC PDE * [Vfetk_PDE_ctor](#) ([Vfetk](#) *fetk)

Constructs the FEtk PDE object.
- VEXTERNC int [Vfetk_PDE_ctor2](#) (PDE *thee, [Vfetk](#) *fetk)

Initializes the FEtk PDE object.
- VEXTERNC void [Vfetk_PDE_dtor](#) (PDE **thee)

Destroys FEtk PDE object.
- VEXTERNC void [Vfetk_PDE_dtor2](#) (PDE *thee)

FORTRAN stub: destroys FEtk PDE object.
- VEXTERNC void [Vfetk_PDE_initAssemble](#) (PDE *thee, int ip[], double rp[])

Do once-per-assembly initialization.
- VEXTERNC void [Vfetk_PDE_initElement](#) (PDE *thee, int elementType, int chart, double txx[][[VAPBS_DIM](#)], void *data)

Do once-per-element initialization.
- VEXTERNC void [Vfetk_PDE_initFace](#) (PDE *thee, int faceType, int chart, double tvec[])

Do once-per-face initialization.
- VEXTERNC void [Vfetk_PDE_initPoint](#) (PDE *thee, int pointType, int chart, double txq[], double tU[], double tdU[][[VAPBS_DIM](#)])

Do once-per-point initialization.
- VEXTERNC void [Vfetk_PDE_Fu](#) (PDE *thee, int key, double F[])

Evaluate strong form of PBE. For interior points, this is:
- VEXTERNC double [Vfetk_PDE_Fu_v](#) (PDE *thee, int key, double V[], double dV[][[VAPBS_DIM](#)])

This is the weak form of the PBE; i.e. the strong form integrated with a test function to give:

- VEXTERNC double [Vfetk_PDE_DFu_wv](#) (PDE *thee, int key, double W[], double dW[][VAPBS_DIM], double V[], double dV[][VAPBS_DIM])
This is the linearization of the weak form of the PBE; e.g., for use in a Newton iteration. This is the functional linearization of the strong form integrated with a test function to give:
- VEXTERNC void [Vfetk_PDE_delta](#) (PDE *thee, int type, int chart, double txq[], void *user, double F[])
Evaluate a (discretized) delta function source term at the given point.
- VEXTERNC void [Vfetk_PDE_u_D](#) (PDE *thee, int type, int chart, double txq[], double F[])
Evaluate the Dirichlet boundary condition at the given point.
- VEXTERNC void [Vfetk_PDE_u_T](#) (PDE *thee, int type, int chart, double txq[], double F[])
Evaluate the "true solution" at the given point for comparison with the numerical solution.
- VEXTERNC void [Vfetk_PDE_bisectEdge](#) (int dim, int dimII, int edgeType, int chart[], double vx[][VAPBS_DIM])
Define the way manifold edges are bisected.
- VEXTERNC void [Vfetk_PDE_mapBoundary](#) (int dim, int dimII, int vertexType, int chart, double vx[VAPBS_DIM])
Map a boundary point to some pre-defined shape.
- VEXTERNC int [Vfetk_PDE_markSimplex](#) (int dim, int dimII, int simplexType, int faceType[VAPBS_NVS], int vertexType[VAPBS_NVS], int chart[], double vx[][VAPBS_DIM], void *simplex)
User-defined error estimator – in our case, a geometry-based refinement method; forcing simplex refinement at the dielectric boundary and (for non-regularized PBE) the charges.
- VEXTERNC void [Vfetk_PDE_oneChart](#) (int dim, int dimII, int objType, int chart[], double vx[][VAPBS_DIM], int dimV)
Unify the chart for different coordinate systems – a no-op for us.
- VEXTERNC double [Vfetk_PDE_Ju](#) (PDE *thee, int key)
Energy functional. This returns the energy (less delta function terms) in the form:
- VEXTERNC void [Vfetk_externalUpdateFunction](#) (SS **simps, int num)
External hook to simplex subdivision routines in Gem. Called each time a simplex is subdivided (we use it to update the charge-simplex map)
- VEXTERNC int [Vfetk_PDE_simplexBasisInit](#) (int key, int dim, int comp, int *ndof, int dof[])
Initialize the bases for the trial or the test space, for a particular component of the system, at all quadrature points on the master simplex element.
- VEXTERNC void [Vfetk_PDE_simplexBasisForm](#) (int key, int dim, int comp, int pdkey, double xq[], double basis[])
Evaluate the bases for the trial or test space, for a particular component of the system, at all quadrature points on the master simplex element.
- VEXTERNC void [Vfetk_readMesh](#) (Vfetk *thee, int skey, Vio *sock)
Read in mesh and initialize associated internal structures.
- VEXTERNC void [Vfetk_dumpLocalVar](#) ()
Debugging routine to print out local variables used by PDE object.
- VEXTERNC int [Vfetk_fillArray](#) (Vfetk *thee, Bvec *vec, Vdata_Type type)
Fill an array with the specified data.
- VEXTERNC int [Vfetk_write](#) (Vfetk *thee, const char *iodev, const char *iofmt, const char *thost, const char *fname, Bvec *vec, Vdata_Format format)
Write out data.
- VEXTERNC Vrc_Codes [Vfetk_loadGem](#) (Vfetk *thee, Gem *gm)
Load a Gem geometry manager object into Vfetk.

9.10.1 Detailed Description

Contains declarations for class Vfetk.

Version

\$Id\$

Author

Nathan A. Baker

Attention

```
*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
*   Nathan A. Baker (nathan.baker@pnnl.gov)
*   Pacific Northwest National Laboratory
*
*   Additional contributing authors listed in the code documentation.
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* ARISING IN ANY WAY OUT OF THE USE OF THIS SOFTWARE, EVEN IF ADVISED OF
* THE POSSIBILITY OF SUCH DAMAGE.
*
*
```

Definition in file [vfetk.h](#).

9.10.2 Typedef Documentation

9.10.2.1 Vfetk

```
typedef struct sVfetk Vfetk
```

Definition at line 207 of file [vfetk.h](#).

9.11 vfetk.h

[Go to the documentation of this file.](#)

```

00001
00062 #ifndef _VFETK_H_
00063 #define _VFETK_H_
00064
00065 #include "apbscfg.h"
00066
00067 #include "malloc/malloc.h"
00068 #include "mc/mc.h"
00069
00070 #include "generic/vhal.h"
00071 #include "generic/vatom.h"
00072 // #include "generic/valist.h"
00073 #include "generic/vpbe.h"
00074 #include "generic/vunit.h"
00075 #include "generic/vgreen.h"
00076 #include "generic/vcap.h"
00077 #include "generic/pbeparm.h"
00078 #include "generic/femparm.h"
00079 #include "fem/vcsm.h"
00080
00086 enum eVfetk_LsolvType {
00087     VLT_SLU=0,
00088     VLT_MG=1,
00089     VLT_CG=2,
00090     VLT_BCG=3
00091 };
00092
00097 typedef enum eVfetk_LsolvType Vfetk_LsolvType;
00098
00099
00104 enum eVfetk_MeshLoad {
00105     VML_DIRICUBE,
00106     VML_NEUMCUBE,
00107     VML_EXTERNAL
00108 };
00109
00114 typedef enum eVfetk_MeshLoad Vfetk_MeshLoad;
00115
00121 enum eVfetk_NsolvType {
00122     VNT_NEW=0,
00123     VNT_INC=1,
00124     VNT_ARC=2
00125 };
00126
00131 typedef enum eVfetk_NsolvType Vfetk_NsolvType;
00132
00138 enum eVfetk_GuessType {
00139     VGT_ZERO=0,
00140     VGT_DIRI=1,
00141     VGT_PREV=2
00142 };
00143
00148 typedef enum eVfetk_GuessType Vfetk_GuessType;
00149
00155 enum eVfetk_PrecType {
00156     VPT_IDEN=0,
00157     VPT_DIAG=1,
00158     VPT_MG=2
00159 };
00160
00165 typedef enum eVfetk_PrecType Vfetk_PrecType;
00166
00176 struct sVfetk {
00177
00178     Vmem *vmem;
00179     Gem *gm;
00182     AM *am;
00183     Aprx *aprx;
00184     PDE *pde;
00185     Vpbe *vpbe;
00186     Vcsm *csm;
00187     Vfetk_LsolvType lkey;
00188     int lmax;

```

```

00189     double ltol;
00190     Vfetk_NsolvType nkey;
00191     int nmax;
00192     double ntol;
00193     Vfetk_GuessType gues;
00194     Vfetk_PrecType lprec;
00195     int pjac;
00197     PBEparm *pbeparm;
00198     FEMParm *feparm;
00199     Vhal_PBEType type;
00200     int level;
00202 };
00203
00207 typedef struct sVfetk Vfetk;
00208
00215 struct sVfetk_LocalVar {
00216     double nvec[VAPBS_DIM];
00217     double vx[4][VAPBS_DIM];
00218     double xq[VAPBS_DIM];
00219     double U[MAXV];
00220     double dU[MAXV][VAPBS_DIM];
00221     double W;
00222     double dW[VAPBS_DIM];
00223     double d2W;
00224     int sType;
00225     int fType;
00226     double diel;
00227     double ionacc;
00228     double A;
00229     double F;
00230     double B;
00231     double DB;
00232     double jumpDiel;
00233     Vfetk *fetk;
00234     Vgreen *green;
00235     int initGreen;
00237     SS *simp;
00239     VV *verts[4];
00240     int nverts;
00241     double ionConc[MAXION];
00242     double ionQ[MAXION];
00243     double ionRadii[MAXION];
00244     double zkappa2;
00245     double zks2;
00246     double ionstr;
00247     int nion;
00248     double Fu_v;
00249     double DFu_wv;
00250     double delta;
00251     double u_D;
00252     double u_T;
00253 };
00254
00259 typedef struct sVfetk_LocalVar Vfetk_LocalVar;
00260
00261 #if !defined(VINLINE_VFETK)
00262
00268     VEXTERNC Gem* Vfetk_getGem(
00269         Vfetk *thee
00270     );
00271
00277     VEXTERNC AM* Vfetk_getAM(
00278         Vfetk *thee
00279     );
00280
00286     VEXTERNC Vpbe* Vfetk_getVpbe(
00287         Vfetk *thee
00288     );
00289
00295     VEXTERNC Vcsm* Vfetk_getVcsm(
00296         Vfetk *thee
00297     );
00298
00305     VEXTERNC int Vfetk_getAtomColor(
00306         Vfetk *thee,
00307         int iatom
00308     );
00309
00310 #else /* if defined(VINLINE_VFETK) */
00311 #     define Vfetk_getGem(thee) ((thee)->gm)
00312 #     define Vfetk_getAM(thee) ((thee)->am)

```

```

00313 #   define Vfetk_getVpbe(thee) ((thee)->pbe)
00314 #   define Vfetk_getVcsm(thee) ((thee)->csm)
00315 #   define Vfetk_getAtomColor(thee, iatom) (Vatom_getPartID(Valist_getAtom(Vpbe_getValist(thee->pbe),
iatom)))
00316 #endif /* if !defined(VINLINE_VFETK) */
00317
00318 /* ////////////////////////////////////// */
00319 // Class Vfetk: Non-Inlineable methods (vfetk.c)
00320
00321
00331 VEXTERNC Vfetk* Vfetk_ctor(
00332     Vpbe *pbe, /**< Vpbe (PBE manager object) */
00333     Vhal_PBEType type
00334 );
00335
00345 VEXTERNC int Vfetk_ctor2(
00346     Vfetk *thee,
00347     Vpbe *pbe,
00348     Vhal_PBEType type
00349 );
00350
00356 VEXTERNC void Vfetk_dtor(
00357     Vfetk **thee
00358 );
00359
00365 VEXTERNC void Vfetk_dtor2(
00366     Vfetk *thee
00367 );
00368
00378 VEXTERNC double* Vfetk_getSolution(
00379     Vfetk *thee,
00380     int *length
00381 );
00382
00388 VEXTERNC void Vfetk_setParameters(
00389     Vfetk *thee,
00390     PBEparm *pbeparm,
00391     FEMparm *feparm
00392 );
00393
00412 VEXTERNC double Vfetk_energy(
00413     Vfetk *thee,
00414     int color,
00418     int nonlin
00420 );
00421
00451 VEXTERNC double Vfetk_dqmEnergy(
00452     Vfetk *thee,
00453     int color
00457 );
00458
00476 VEXTERNC double Vfetk_qfEnergy(
00477     Vfetk *thee,
00478     int color
00480 );
00481
00489 VEXTERNC unsigned long int Vfetk_memChk(
00490     Vfetk *thee
00491 );
00492
00508 VEXTERNC void Vfetk_setAtomColors(
00509     Vfetk *thee
00510 );
00511
00520 VEXTERNC void Bmat_printHB(
00521     Bmat *thee,
00522     char *fname
00523 );
00524
00530 VEXTERNC Vrc_Codes Vfetk_genCube(
00531     Vfetk *thee,
00532     double center[3],
00533     double length[3],
00534     Vfetk_MeshLoad meshType
00535 );
00536
00542 VEXTERNC Vrc_Codes Vfetk_loadMesh(
00543     Vfetk *thee,
00544     double center[3],
00545     double length[3],
00546     Vfetk_MeshLoad meshType,
00547     Vio *sock

```



```

00548                                     );
00549
00556 VEXTERNC PDE* Vfetk_PDE_ctor(
00557     Vfetk *fetk
00558 );
00559
00566 VEXTERNC int Vfetk_PDE_ctor2(
00567     PDE *thee,
00568     Vfetk *fetk
00569 );
00570
00577 VEXTERNC void Vfetk_PDE_dtor(
00578     PDE **thee
00579 );
00580
00587 VEXTERNC void Vfetk_PDE_dtor2(
00588     PDE *thee
00589 );
00590
00596 VEXTERNC void Vfetk_PDE_initAssemble(
00597     PDE *thee,
00598     int ip[],
00599     double rp[]
00600 );
00601
00608 VEXTERNC void Vfetk_PDE_initElement(
00609     PDE *thee,
00610     int elementType,
00611     int chart,
00614     double tvx[][VAPBS_DIM],
00615     void *data
00616 );
00617
00623 VEXTERNC void Vfetk_PDE_initFace(
00624     PDE *thee,
00625     int faceType,
00627     int chart,
00629     double tnvec[]
00630 );
00631
00639 VEXTERNC void Vfetk_PDE_initPoint(
00640     PDE *thee,
00641     int pointType,
00642     int chart,
00644     double txq[],
00645     double tU[],
00646     double tdU[][VAPBS_DIM]
00647 );
00648
00666 VEXTERNC void Vfetk_PDE_Fu(
00667     PDE *thee,
00668     int key,
00670     double F[]
00671 );
00672
00683 VEXTERNC double Vfetk_PDE_Fu_v(
00684     PDE *thee,
00685     int key,
00687     double V[],
00688     double dv[][VAPBS_DIM]
00689 );
00690
00702 VEXTERNC double Vfetk_PDE_DFu_wv(
00703     PDE *thee,
00704     int key,
00706     double W[],
00707     double dW[][VAPBS_DIM],
00708     double V[],
00709     double dv[][VAPBS_DIM]
00710 );
00711
00718 VEXTERNC void Vfetk_PDE_delta(
00719     PDE *thee,
00720     int type,
00721     int chart,
00722     double txq[],
00723     void *user,
00724     double F[]
00725 );
00726
00734 VEXTERNC void Vfetk_PDE_u_D(

```

```

00735         PDE *thee,
00736         int type,
00737         int chart,
00738         double txq[],
00739         double F[]
00740     );
00741
00749 VEXTERNC void Vfetk_PDE_u_T(
00750     PDE *thee,
00751     int type,
00752     int chart,
00753     double txq[],
00754     double F[]
00755 );
00756
00762 VEXTERNC void Vfetk_PDE_bisectEdge(
00763     int dim,
00764     int dimII,
00765     int edgeType,
00766     int chart[],
00768     double vx[][VAPBS_DIM]
00769 );
00770
00776 VEXTERNC void Vfetk_PDE_mapBoundary(
00777     int dim,
00778     int dimII,
00779     int vertexType,
00780     int chart,
00781     double vx[VAPBS_DIM]
00782 );
00783
00792 VEXTERNC int Vfetk_PDE_markSimplex(
00793     int dim,
00794     int dimII,
00795     int simplexType,
00796     int faceType[VAPBS_NVS],
00797     int vertexType[VAPBS_NVS],
00798     int chart[],
00799     double vx[][VAPBS_DIM],
00800     void *simplex
00801 );
00802
00808 VEXTERNC void Vfetk_PDE_oneChart(
00809     int dim,
00810     int dimII,
00811     int objType,
00812     int chart[],
00813     double vx[][VAPBS_DIM],
00814     int dimV
00815 );
00816
00826 VEXTERNC double Vfetk_PDE_Ju(
00827     PDE *thee,
00828     int key
00829 );
00830
00838 VEXTERNC void Vfetk_externalUpdateFunction(
00839     SS **simps,
00841     int num
00842 );
00843
00844
00907 VEXTERNC int Vfetk_PDE_simplexBasisInit(
00908     int key,
00910     int dim,
00911     int comp,
00913     int *ndof,
00914     int dof[]
00915 );
00916
00924 VEXTERNC void Vfetk_PDE_simplexBasisForm(
00925     int key,
00927     int dim,
00928     int comp ,
00929     int pdkey,
00938     double xq[],
00939     double basis[]
00941 );
00942
00948 VEXTERNC void Vfetk_readMesh(
00949     Vfetk *thee,

```

```

00950         int skey,
00951         Vio *sock
00952     );
00953
00959 VEXTERNC void Vfetc_dumpLocalVar();
00960
00968 VEXTERNC int Vfetc_fillArray(
00969     Vfetc *thee,
00970     Bvec *vec,
00971     Vdata_Type type
00972 );
00973
00988 VEXTERNC int Vfetc_write(
00989     Vfetc *thee,
00990     const char *iodev,
00992     const char *iofmt,
00994     const char *thost,
00995     const char *fname,
00996     Bvec *vec,
00997     Vdata_Format format
00998 );
00999
01005 VEXTERNC Vrc_Codes Vfetc_loadGem(
01006     Vfetc *thee,
01007     Gem *gm
01008 );
01009
01010
01011 #endif /* ifndef _VFETK_H_ */

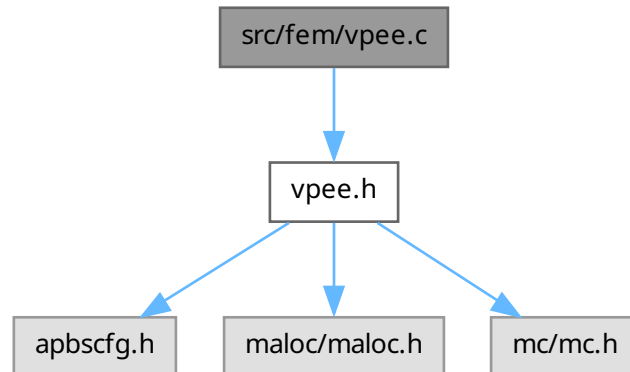
```

9.12 src/fem/vpee.c File Reference

Class Vpee methods.

```
#include "vpee.h"
```

Include dependency graph for vpee.c:



Functions

- VPRIVATE int **Vpee_userDefined** (Vpee *thee, SS *sm)
- VPRIVATE int **Vpee_ourSimp** (Vpee *thee, SS *sm, int rcol)
- VEXTERNC double **Aprx_estNonlinResid** (Aprx *thee, SS *sm, Bvec *u, Bvec *ud, Bvec *f)
- VEXTERNC double **Aprx_estLocalProblem** (Aprx *thee, SS *sm, Bvec *u, Bvec *ud, Bvec *f)

- VEXTERNC double **Aprx_estDualProblem** (Aprx *thee, SS *sm, Bvec *u, Bvec *ud, Bvec *f)
- VPUBLIC Vpee * **Vpee_ctor** (Gem *gm, int localPartID, int killFlag, double killParam)
Construct the Vpee object.
- VPUBLIC int **Vpee_ctor2** (Vpee *thee, Gem *gm, int localPartID, int killFlag, double killParam)
FORTTRAN stub to construct the Vpee object.
- VPUBLIC void **Vpee_dtor** (Vpee **thee)
Object destructor.
- VPUBLIC void **Vpee_dtor2** (Vpee *thee)
FORTTRAN stub object destructor.
- VPUBLIC int **Vpee_markRefine** (Vpee *thee, AM *am, int level, int akey, int rcol, double etol, int bkey)
Mark simplices for refinement based on attenuated error estimates.
- VPUBLIC int **Vpee_numSS** (Vpee *thee)
Returns the number of simplices in the local partition.

9.12.1 Detailed Description

Class Vpee methods.

Author

Nathan Baker

Version

\$Id\$

Attention

```
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* APBS -- Adaptive Poisson-Boltzmann Solver
*
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*
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```

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*
*

```

Definition in file [vpee.c](#).

9.12.2 Function Documentation

9.12.2.1 Vpee_ourSimp()

```

VPRIVATE int Vpee_ourSimp (
    Vpee * thee,
    SS * sm,
    int rcol )

```

Definition at line 532 of file [vpee.c](#).

9.12.2.2 Vpee_userDefined()

```

VPRIVATE int Vpee_userDefined (
    Vpee * thee,
    SS * sm )

```

Definition at line 498 of file [vpee.c](#).

9.13 vpee.c

[Go to the documentation of this file.](#)

```

00001
00057 #include "vpee.h"
00058
00059 VPRIVATE int Vpee_userDefined(Vpee *thee,
00060                               SS *sm
00061                               );
00062 VPRIVATE int Vpee_ourSimp(Vpee *thee,
00063                           SS *sm,
00064                           int rcol
00065                           );
00066 VEXTERNC double Aprx_estNonlinResid(Aprx *thee,
00067                                     SS *sm,
00068                                     Bvec *u,
00069                                     Bvec *ud,
00070                                     Bvec *f
00071                                     );
00072 VEXTERNC double Aprx_estLocalProblem(Aprx *thee,
00073                                      SS *sm,
00074                                      Bvec *u,
00075                                      Bvec *ud,
00076                                      Bvec *f);
00077 VEXTERNC double Aprx_estDualProblem(Aprx *thee,
00078                                     SS *sm,
00079                                     Bvec *u,
00080                                     Bvec *ud,
00081                                     Bvec *f
00082                                     );
00083
00084 /* ////////////////////////////////////////
00085 // Class Vpee: Non-inlineable methods

```

```

00087
00088 /* ////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////// */
00089 // Routine: Vpee_ctor
00090 //
00091 // Author: Nathan Baker
00093 VPUBLIC Vpee* Vpee_ctor(Gem *gm,
00094                        int localPartID,
00095                        int killFlag,
00096                        double killParam
00097                        ) {
00098
00099     Vpee *thee = VNULL;
00100
00101     /* Set up the structure */
00102     thee = Vmem_malloc(VNULL, 1, sizeof(Vpee) );
00103     VASSERT( thee != VNULL);
00104     VASSERT( Vpee_ctor2(thee, gm, localPartID, killFlag, killParam));
00105
00106     return thee;
00107 }
00108
00109 /* ////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////// */
00110 // Routine: Vpee_ctor2
00111 //
00112 // Author: Nathan Baker
00114 VPUBLIC int Vpee_ctor2(Vpee *thee,
00115                      Gem *gm,
00116                      int localPartID,
00117                      int killFlag,
00118                      double killParam
00119                      ) {
00120
00121     int ivert,
00122         nLocalVerts;
00123     SS *simp;
00124     VV *vert;
00125     double radius,
00126         dx,
00127         dy,
00128         dz;
00129
00130     VASSERT(thee != VNULL);
00131
00132     /* Sanity check on input values */
00133     if (killFlag == 0) {
00134         Vnm_print(0, "Vpee_ctor2: No error attenuation outside partition.\n");
00135     } else if (killFlag == 1) {
00136         Vnm_print(0, "Vpee_ctor2: Error outside local partition ignored.\n");
00137     } else if (killFlag == 2) {
00138         Vnm_print(0, "Vpee_ctor2: Error ignored outside sphere with radius %4.3f times the radius of the
00139 circumscribing sphere\n", killParam);
00140         if (killParam < 1.0) {
00141             Vnm_print(2, "Vpee_ctor2: Warning! Parameter killParam = %4.3 < 1.0!\n",
00142                 killParam);
00143             Vnm_print(2, "Vpee_ctor2: This may result in non-optimal marking and refinement!\n");
00144         }
00145     } else if (killFlag == 3) {
00146         Vnm_print(0, "Vpee_ctor2: Error outside local partition and immediate neighbors ignored [NOT
00147 IMPLEMENTED].\n");
00148     } else {
00149         Vnm_print(2, "Vpee_ctor2: UNRECOGNIZED killFlag PARAMETER! BAILING!\n");
00150         VASSERT(0);
00151     }
00152
00153     thee->gm = gm;
00154     thee->localPartID = localPartID;
00155     thee->killFlag = killFlag;
00156     thee->killParam = killParam;
00157     thee->mem = Vmem_ctor("APBS::VPEE");
00158
00159     /* Now, figure out the center of geometry for the local partition. The
00160      * general plan is to loop through the vertices, loop through the
00161      * vertices' simplex lists and find the vertices with simplices containing
00162      * chart values we're interested in. */
00163     thee->localPartCenter[0] = 0.0;
00164     thee->localPartCenter[1] = 0.0;
00165     thee->localPartCenter[2] = 0.0;
00166     nLocalVerts = 0;
00167     for (ivert=0; ivert<Gem_numVV(thee->gm); ivert++) {
00168         vert = Gem_VV(thee->gm, ivert);
00169         simp = VV_firstSS(vert);

```

```

00168     VASSERT(simp != VNULL);
00169     while (simp != VNULL) {
00170         if (SS_chart(simp) == thee->localPartID) {
00171             thee->localPartCenter[0] += VV_coord(vert, 0);
00172             thee->localPartCenter[1] += VV_coord(vert, 1);
00173             thee->localPartCenter[2] += VV_coord(vert, 2);
00174             nLocalVerts++;
00175             break;
00176         }
00177         simp = SS_link(simp, vert);
00178     }
00179 }
00180 VASSERT(nLocalVerts > 0);
00181 thee->localPartCenter[0] =
00182     thee->localPartCenter[0]/((double)(nLocalVerts));
00183 thee->localPartCenter[1] =
00184     thee->localPartCenter[1]/((double)(nLocalVerts));
00185 thee->localPartCenter[2] =
00186     thee->localPartCenter[2]/((double)(nLocalVerts));
00187 Vnm_print(0, "Vpee_ctor2: Part %d centered at (%4.3f, %4.3f, %4.3f)\n",
00188     thee->localPartID, thee->localPartCenter[0], thee->localPartCenter[1],
00189     thee->localPartCenter[2]);
00190
00191
00192 /* Now, figure out the radius of the sphere circumscribing the local
00193  * partition. We need to keep track of vertices so we don't double count
00194  * them. */
00195 thee->localPartRadius = 0.0;
00196 for (ivert=0; ivert<Gem_numVV(thee->gm); ivert++) {
00197     vert = Gem_VV(thee->gm, ivert);
00198     simp = VV_firstSS(vert);
00199     VASSERT(simp != VNULL);
00200     while (simp != VNULL) {
00201         if (SS_chart(simp) == thee->localPartID) {
00202             dx = thee->localPartCenter[0] - VV_coord(vert, 0);
00203             dy = thee->localPartCenter[1] - VV_coord(vert, 1);
00204             dz = thee->localPartCenter[2] - VV_coord(vert, 2);
00205             radius = dx*dx + dy*dy + dz*dz;
00206             if (radius > thee->localPartRadius) thee->localPartRadius =
00207                 radius;
00208             break;
00209         }
00210         simp = SS_link(simp, vert);
00211     }
00212 }
00213 thee->localPartRadius = VSQRT(thee->localPartRadius);
00214 Vnm_print(0, "Vpee_ctor2: Part %d has circumscribing sphere of radius %4.3f\n",
00215     thee->localPartID, thee->localPartRadius);
00216
00217 return 1;
00218 }
00219
00220 /* ////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////
00221 // Routine: Vpee_dtor
00222 //
00223 // Author: Nathan Baker
00225 VPUBLIC void Vpee_dtor(Vpee **thee) {
00226
00227     if ((*thee) != VNULL) {
00228         Vpee_dtor2(*thee);
00229         Vmem_free(VNULL, 1, sizeof(Vpee), (void **)thee);
00230         (*thee) = VNULL;
00231     }
00232 }
00233 }
00234
00235 /* ////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////
00236 // Routine: Vpee_dtor2
00237 //
00238 // Author: Nathan Baker
00240 VPUBLIC void Vpee_dtor2(Vpee *thee) {
00241     Vmem_dtor(&(thee->mem));
00242 }
00243
00244 /* ////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////
00245 // Routine: Vpee_markRefine
00246 //
00247 // Author: Nathan Baker (and Michael Holst: the author of AM_markRefine, on
00248 // which this is based)
00250 VPUBLIC int Vpee_markRefine(Vpee *thee,
00251     AM *am,

```

```

00252             int level,
00253             int akey,
00254             int rcol,
00255             double etol,
00256             int bkey
00257         ) {
00258
00259     Aprx *aprx;
00260     int marked = 0,
00261         markMe,
00262         i,
00263         smid,
00264         count,
00265         currentQ;
00266     double minError = 0.0,
00267         maxError = 0.0,
00268         errEst = 0.0,
00269         mlevel,
00270         barrier;
00271     SS *sm;
00272
00273     VASSERT(thee != VNULL);
00274
00275     /* Get the Aprx object from AM */
00276     aprx = am->aprx;
00277
00278     /* input check and some i/o */
00279     if ( ! ((-1 <= akey) && (akey <= 4)) ) {
00280         Vnm_print(0, "Vpee_markRefine: bad refine key; simplices marked = %d\n",
00281             marked);
00282         return marked;
00283     }
00284
00285     /* For uniform markings, we have no effect */
00286     if ((-1 <= akey) && (akey <= 0)) {
00287         marked = Gem_markRefine(thee->gm, akey, rcol);
00288         return marked;
00289     }
00290
00291     /* Informative I/O */
00292     if (akey == 2) {
00293         Vnm_print(0, "Vpee_estRefine: using Aprx_estNonlinResid().\n");
00294     } else if (akey == 3) {
00295         Vnm_print(0, "Vpee_estRefine: using Aprx_estLocalProblem().\n");
00296     } else if (akey == 4) {
00297         Vnm_print(0, "Vpee_estRefine: using Aprx_estDualProblem().\n");
00298     } else {
00299         Vnm_print(0, "Vpee_estRefine: bad key given; simplices marked = %d\n",
00300             marked);
00301         return marked;
00302     }
00303
00304     if (thee->killFlag == 0) {
00305         Vnm_print(0, "Vpee_markRefine: No error attenuation -- simplices in all partitions will be
marked.\n");
00306     } else if (thee->killFlag == 1) {
00307         Vnm_print(0, "Vpee_markRefine: Maximum error attenuation -- only simplices in local partition will
be marked.\n");
00308     } else if (thee->killFlag == 2) {
00309         Vnm_print(0, "Vpee_markRefine: Spherical error attenuation -- simplices within a sphere of %4.3f
times the size of the partition will be marked\n",
00310             thee->killParam);
00311     } else if (thee->killFlag == 2) {
00312         Vnm_print(0, "Vpee_markRefine: Neighbor-based error attenuation -- simplices in the local and
neighboring partitions will be marked [NOT IMPLEMENTED]!\n");
00313         VASSERT(0);
00314     } else {
00315         Vnm_print(2, "Vpee_markRefine: bogus killFlag given; simplices marked = %d\n",
00316             marked);
00317         return marked;
00318     }
00319
00320     /* set the barrier type */
00321     mlevel = (etol*etol) / Gem_numSS(thee->gm);
00322     if (bkey == 0) {
00323         barrier = (etol*etol);
00324         Vnm_print(0, "Vpee_estRefine: forcing [err per S] < [TOL] = %g\n",
00325             barrier);
00326     } else if (bkey == 1) {
00327         barrier = mlevel;
00328         Vnm_print(0, "Vpee_estRefine: forcing [err per S] < [(TOL^2/numS)^(1/2)] = %g\n",

```



```

00329         VSQRT(barrier));
00330     } else {
00331         Vnm_print(0,"Vpee_estRefine: bad bkey given; simplices marked = %d\n",
00332             marked);
00333         return marked;
00334     }
00335
00336     /* timer */
00337     Vnm_tstart(30, "error estimation");
00338
00339     /* count = num generations to produce from marked simplices (minimally) */
00340     count = 1; /* must be >= 1 */
00341
00342     /* check the refinement Q for emptiness */
00343     currentQ = 0;
00344     if (Gem_numSQ(thee->gm,currentQ) > 0) {
00345         Vnm_print(0,"Vpee_markRefine: non-empty refinement Q%d....clearing..",
00346             currentQ);
00347         Gem_resetSQ(thee->gm,currentQ);
00348         Vnm_print(0,"..done.\n");
00349     }
00350     if (Gem_numSQ(thee->gm,!currentQ) > 0) {
00351         Vnm_print(0,"Vpee_markRefine: non-empty refinement Q%d....clearing..",
00352             !currentQ);
00353         Gem_resetSQ(thee->gm,!currentQ);
00354         Vnm_print(0,"..done.\n");
00355     }
00356     VASSERT( Gem_numSQ(thee->gm,currentQ) == 0 );
00357     VASSERT( Gem_numSQ(thee->gm,!currentQ) == 0 );
00358
00359     /* clear everyone's refinement flags */
00360     Vnm_print(0,"Vpee_markRefine: clearing all simplex refinement flags..");
00361     for (i=0; i<Gem_numSS(thee->gm); i++) {
00362         if ( (i>0) && (i % VPRTKEY) == 0 ) Vnm_print(0,"[MS:%d]",i);
00363         sm = Gem_SS(thee->gm,i);
00364         SS_setRefineKey(sm,currentQ,0);
00365         SS_setRefineKey(sm,!currentQ,0);
00366         SS_setRefinementCount(sm,0);
00367     }
00368     Vnm_print(0,"..done.\n");
00369
00370     /* NON-ERROR-BASED METHODS */
00371     /* Simplex flag clearing */
00372     if (akey == -1) return marked;
00373     /* Uniform & user-defined refinement*/
00374     if ((akey == 0) || (akey == 1)) {
00375         smid = 0;
00376         while ( smid < Gem_numSS(thee->gm) ) {
00377             /* Get the simplex and find out if it's markable */
00378             sm = Gem_SS(thee->gm,smid);
00379             markMe = Vpee_ourSimp(thee, sm, rcol);
00380             if (markMe) {
00381                 if (akey == 0) {
00382                     marked++;
00383                     Gem_appendSQ(thee->gm,currentQ, sm);
00384                     SS_setRefineKey(sm,currentQ,1);
00385                     SS_setRefinementCount(sm,count);
00386                 } else if (Vpee_userDefined(thee, sm)) {
00387                     marked++;
00388                     Gem_appendSQ(thee->gm,currentQ, sm);
00389                     SS_setRefineKey(sm,currentQ,1);
00390                     SS_setRefinementCount(sm,count);
00391                 }
00392             }
00393             smid++;
00394         }
00395     }
00396
00397     /* ERROR-BASED METHODS */
00398     /* gerror = global error accumulation */
00399     aprx->gerror = 0.;
00400
00401     /* traverse the simplices and process the error estimates */
00402     Vnm_print(0,"Vpee_markRefine: estimating error..");
00403     smid = 0;
00404     while ( smid < Gem_numSS(thee->gm) ) {
00405
00406         /* Get the simplex and find out if it's markable */
00407         sm = Gem_SS(thee->gm,smid);
00408         markMe = Vpee_ourSimp(thee, sm, rcol);
00409     }

```

```

00410         if ( (smid>0) && (smid % VPRTKEY) == 0 ) Vnm_print(0,"[MS:%d]",smid);
00411
00412         /* Produce an error estimate for this element if it is in the set */
00413         if (markMe) {
00414             if (akey == 2) {
00415                 errEst = Aprx_estNonlinResid(aprx, sm, am->u,am->ud,am->f);
00416             } else if (akey == 3) {
00417                 errEst = Aprx_estLocalProblem(aprx, sm, am->u,am->ud,am->f);
00418             } else if (akey == 4) {
00419                 errEst = Aprx_estDualProblem(aprx, sm, am->u,am->ud,am->f);
00420             }
00421             VASSERT( errEst >= 0. );
00422
00423             /* if error estimate above tol, mark element for refinement */
00424             if ( errEst > barrier ) {
00425                 marked++;
00426                 Gem_appendSQ(thee->gm,currentQ, sm); /*add to refinement Q*/
00427                 SS_setRefineKey(sm,currentQ,1);      /* note now on refine Q */
00428                 SS_setRefinementCount(sm,count);      /* refine X many times? */
00429             }
00430
00431             /* keep track of min/max errors over the mesh */
00432             minError = VMIN2( VSQRT(VABS(errEst)), minError );
00433             maxError = VMAX2( VSQRT(VABS(errEst)), maxError );
00434
00435             /* store the estimate */
00436             Bvec_set( aprx->wev, smid, errEst );
00437
00438             /* accumulate into global error (errEst is SQUARED already) */
00439             aprx->gerror += errEst;
00440
00441             /* otherwise store a zero for the estimate */
00442             } else {
00443                 Bvec_set( aprx->wev, smid, 0. );
00444             }
00445
00446             smid++;
00447         }
00448
00449         /* do some i/o */
00450         Vnm_print(0,"..done. [marked=<%d/%d>]\n",marked,Gem_numSS(thee->gm));
00451         Vnm_print(0,"Vpee_estRefine: TOL=<%g> Global_Error=<%g>\n",
00452             etol, aprx->gerror);
00453         Vnm_print(0,"Vpee_estRefine: (TOL^2/numS)^(1/2)=<%g> Max_Ele_Error=<%g>\n",
00454             VSQRT(mlevel),maxError);
00455         Vnm_tstop(30, "error estimation");
00456
00457         /* check for making the error tolerance */
00458         if ((bkey == 1) && (aprx->gerror <= etol)) {
00459             Vnm_print(0,
00460                 "Vpee_estRefine: *****\n");
00461             Vnm_print(0,
00462                 "Vpee_estRefine: Global Error criterion met; setting marked=0.\n");
00463             Vnm_print(0,
00464                 "Vpee_estRefine: *****\n");
00465             marked = 0;
00466         }
00467
00468         /* return */
00469         return marked;
00470     }
00471 }
00472
00473
00474 /* ////////////////////////////////////////
00475 // Routine: Vpee_numSS
00476 //
00477 // Author: Nathan Baker
00479 VPUBLIC int Vpee_numSS(Vpee *thee) {
00480     int num = 0;
00481     int isimp;
00482
00483     for (isimp=0; isimp<Gem_numSS(thee->gm); isimp++) {
00484         if (SS_chart(Gem_SS(thee->gm, isimp)) == thee->localPartID) num++;
00485     }
00486
00487     return num;
00488 }
00489
00490 /* ////////////////////////////////////////
00491 // Routine: Vpee_userDefined

```

```

00492 //
00493 // Purpose: Reduce code bloat by wrapping up the common steps for getting the
00494 //           user-defined error estimate
00495 //
00496 // Author:   Nathan Baker
00498 VPRIVATE int Vpee_userDefined(Vpee *thee,
00499                               SS *sm
00500                               ) {
00501
00502     int ivert,
00503         icoord,
00504         chart[4],
00505         fType[4],
00506         vType[4];
00507     double vx[4][3];
00508
00509     for (ivert=0; ivert<Gem_dimVV(thee->gm); ivert++) {
00510         fType[ivert] = SS_faceType(sm,ivert);
00511         vType[ivert] = VV_type(SS_vertex(sm,ivert) );
00512         chart[ivert] = VV_chart(SS_vertex(sm,ivert) );
00513         for (icoord=0; icoord<Gem_dimII(thee->gm); icoord++) {
00514             vx[ivert][icoord] = VV_coord(SS_vertex(sm,ivert), icoord );
00515         }
00516     }
00517     return thee->gm->pde->markSimplex(Gem_dim(thee->gm), Gem_dimII(thee->gm),
00518                                     SS_type(sm), fType, vType, chart, vx, sm);
00519 }
00520
00521 /* ////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////
00522 // Routine: Vpee_ourSimp
00523 //
00524 // Purpose: Reduce code bloat by wrapping up the common steps for determining
00525 //           whether the given simplex can be marked (i.e., belongs to our
00526 //           partition or overlap region)
00527 //
00528 // Returns: 1 if could be marked, 0 otherwise
00529 //
00530 // Author:   Nathan Baker
00532 VPRIVATE int Vpee_ourSimp(Vpee *thee,
00533                           SS *sm,
00534                           int rcol
00535                           ) {
00536
00537     int ivert;
00538     double dist,
00539         dx,
00540         dy,
00541         dz;
00542
00543     if (thee->killFlag == 0) return 1;
00544     else if (thee->killFlag == 1) {
00545         if ((SS_chart(sm) == rcol) || (rcol < 0)) return 1;
00546     } else if (thee->killFlag == 2) {
00547         if (rcol < 0) return 1;
00548         else {
00549             /* We can only do distance-based searches on the local partition */
00550             VASSERT(rcol == thee->localPartID);
00551             /* Find the closest distance between this simplex and the
00552              * center of the local partition and check it against
00553              * (thee->localPartRadius*thee->killParam) */
00554             dist = 0;
00555             for (ivert=0; ivert<SS_dimVV(sm); ivert++) {
00556                 dx = VV_coord(SS_vertex(sm, ivert), 0) -
00557                     thee->localPartCenter[0];
00558                 dy = VV_coord(SS_vertex(sm, ivert), 1) -
00559                     thee->localPartCenter[1];
00560                 dz = VV_coord(SS_vertex(sm, ivert), 2) -
00561                     thee->localPartCenter[2];
00562                 dist = VSQRT((dx*dx + dy*dy + dz*dz));
00563             }
00564             if (dist < thee->localPartRadius*thee->killParam) return 1;
00565         }
00566     } else if (thee->killFlag == 3) VASSERT(0);
00567     else VASSERT(0);
00568
00569     return 0;
00570
00571 }

```

9.14 src/fem/vpee.h File Reference

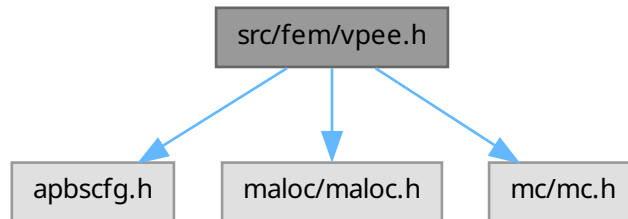
Contains declarations for class Vpee.

```
#include "apbscfg.h"
```

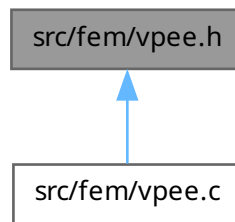
```
#include "maloc/maloc.h"
```

```
#include "mc/mc.h"
```

Include dependency graph for vpee.h:



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [sVpee](#)

Contains public data members for Vpee class/module.

Typedefs

- typedef struct [sVpee](#) [Vpee](#)

Declaration of the Vpee class as the Vpee structure.

Functions

- VEXTERNC [Vpee](#) * [Vpee_ctor](#) (Gem *gm, int localPartID, int killFlag, double killParam)

Construct the Vpee object.

- VEXTERNC int `Vpee_ctor2` (`Vpee *thee`, `Gem *gm`, `int localPartID`, `int killFlag`, `double killParam`)

FORTTRAN stub to construct the Vpee object.

- VEXTERNC void `Vpee_dtor` (`Vpee **thee`)

Object destructor.

- VEXTERNC void `Vpee_dtor2` (`Vpee *thee`)

FORTTRAN stub object destructor.

- VEXTERNC int `Vpee_markRefine` (`Vpee *thee`, `AM *am`, `int level`, `int akey`, `int rcol`, `double etol`, `int bkey`)

Mark simplices for refinement based on attenuated error estimates.

- VEXTERNC int `Vpee_numSS` (`Vpee *thee`)

Returns the number of simplices in the local partition.

9.14.1 Detailed Description

Contains declarations for class `Vpee`.

Version

\$Id\$

Author

Nathan A. Baker

Attention

```
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* APBS -- Adaptive Poisson-Boltzmann Solver
*
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* Pacific Northwest National Laboratory
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*
*

```

Definition in file [vpee.h](#).

9.15 vpee.h

[Go to the documentation of this file.](#)

```

00001
00076 #ifndef _VP EE_H
00077 #define _VP EE_H
00078
00079 #include "apbscfg.h"
00080
00081 #include "malloc/malloc.h"
00082 #include "mc/mc.h"
00083
00089 struct sVpee {
00090
00091     Gem *gm;
00092     int localPartID;
00095     double localPartCenter[3];
00097     double localPartRadius;
00099     int killFlag;
00102     double killParam;
00104     Vmem *mem;
00106 };
00107
00112 typedef struct sVpee Vpee;
00113
00114 /* ////////////////////////////////////////
00115 // Class Vpee Inlineable methods
00117
00118 #if !defined(VINLINE_VPEE)
00119 #else /* if defined(VINLINE_VPEE) */
00120 #endif /* if !defined(VINLINE_VPEE) */
00121
00122 /* ////////////////////////////////////////
00123 // Class Vpee: Non-Inlineable methods (vpee.c)
00125
00132 VEXTERNC Vpee* Vpee_ctor(
00133     Gem *gm, /**< FEtk geometry manager object */
00134     int localPartID,
00135     int killFlag,
00146     double killParam
00147 );
00148
00155 VEXTERNC int Vpee_ctor2(
00156     Vpee *thee,
00157     Gem *gm,
00158     int localPartID,
00159     int killFlag,
00170     double killParam
00171 );
00172
00177 VEXTERNC void Vpee_dtor(
00178     Vpee **thee
00179 );
00180
00185 VEXTERNC void Vpee_dtor2(
00186     Vpee *thee
00187 );
00188
00204 VEXTERNC int Vpee_markRefine(
00205     Vpee *thee,
00206     AM *am,

```

```

00207         int level,
00208         int akey,
00216         int rcol,
00219         double etol,
00220         int bkey
00224     );
00225
00231 VEXTERNC int Vpee_numSS(
00232     Vpee *thee
00233 );
00234
00235 #endif      /* ifndef _VPEE_H_ */

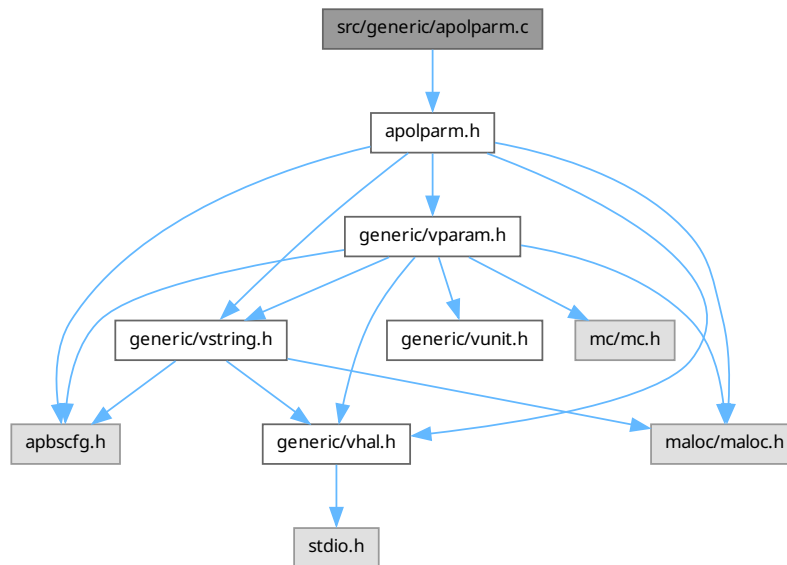
```

9.16 src/generic/apolparm.c File Reference

Class APOLparm methods.

```
#include "apolparm.h"
```

Include dependency graph for apolparm.c:



Functions

- VPUBLIC APOLparm * APOLparm_ctor ()
Construct APOLparm.
- VPUBLIC Vrc_Codes APOLparm_ctor2 (APOLparm *thee)
FORTTRAN stub to construct APOLparm.
- VPUBLIC void APOLparm_copy (APOLparm *thee, APOLparm *source)
Copy target object into thee.
- VPUBLIC void APOLparm_dtor (APOLparm **thee)
Object destructor.
- VPUBLIC void APOLparm_dtor2 (APOLparm *thee)
FORTTRAN stub for object destructor.
- VPUBLIC Vrc_Codes APOLparm_check (APOLparm *thee)

Consistency check for parameter values stored in object.

- VPRIVATE Vrc_Codes [APOLparm_parseGRID](#) (APOLparm *thee, Vio *sock)
- VPRIVATE Vrc_Codes [APOLparm_parseMOL](#) (APOLparm *thee, Vio *sock)
- VPRIVATE Vrc_Codes [APOLparm_parseSRFM](#) (APOLparm *thee, Vio *sock)
- VPRIVATE Vrc_Codes [APOLparm_parseSRAD](#) (APOLparm *thee, Vio *sock)
- VPRIVATE Vrc_Codes [APOLparm_parseSWIN](#) (APOLparm *thee, Vio *sock)
- VPRIVATE Vrc_Codes [APOLparm_parseTEMP](#) (APOLparm *thee, Vio *sock)
- VPRIVATE Vrc_Codes [APOLparm_parseGAMMA](#) (APOLparm *thee, Vio *sock)
- VPRIVATE Vrc_Codes [APOLparm_parseCALCENERGY](#) (APOLparm *thee, Vio *sock)
- VPRIVATE Vrc_Codes [APOLparm_parseCALCFORCE](#) (APOLparm *thee, Vio *sock)
- VPRIVATE Vrc_Codes [APOLparm_parseBCONC](#) (APOLparm *thee, Vio *sock)
- VPRIVATE Vrc_Codes [APOLparm_parseSDENS](#) (APOLparm *thee, Vio *sock)
- VPRIVATE Vrc_Codes [APOLparm_parseDPOS](#) (APOLparm *thee, Vio *sock)
- VPRIVATE Vrc_Codes [APOLparm_parsePRESS](#) (APOLparm *thee, Vio *sock)
- VPUBLIC Vrc_Codes [APOLparm_parseToken](#) (APOLparm *thee, char tok[VMAX_BUFSIZE], Vio *sock)

Parse an MG keyword from an input file.

9.16.1 Detailed Description

Class APOLparm methods.

Author

David Gohara

Version

\$Id\$

Attention

```
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```

Definition in file [apolparm.c](#).

9.16.2 Function Documentation

9.16.2.1 APOLparm_parseBCONC()

```

VPRIVATE Vrc_Codes APOLparm_parseBCONC (
    APOLparm * thee,
    Vio * sock )

```

Definition at line 491 of file [apolparm.c](#).

9.16.2.2 APOLparm_parseCALCENERGY()

```

VPRIVATE Vrc_Codes APOLparm_parseCALCENERGY (
    APOLparm * thee,
    Vio * sock )

```

Definition at line 385 of file [apolparm.c](#).

9.16.2.3 APOLparm_parseCALCFORCE()

```

VPRIVATE Vrc_Codes APOLparm_parseCALCFORCE (
    APOLparm * thee,
    Vio * sock )

```

Definition at line 438 of file [apolparm.c](#).

9.16.2.4 APOLparm_parseDPOS()

```

VPRIVATE Vrc_Codes APOLparm_parseDPOS (
    APOLparm * thee,
    Vio * sock )

```

Definition at line 529 of file [apolparm.c](#).

9.16.2.5 APOLparm_parseGAMMA()

```

VPRIVATE Vrc_Codes APOLparm_parseGAMMA (
    APOLparm * thee,
    Vio * sock )

```

Definition at line 366 of file [apolparm.c](#).

9.16.2.6 APOLparm_parseGRID()

```
VPRIVATE Vrc_Codes APOLparm_parseGRID (  
    APOLparm * thee,  
    Vio * sock )
```

Definition at line 237 of file [apolparm.c](#).

9.16.2.7 APOLparm_parseMOL()

```
VPRIVATE Vrc_Codes APOLparm_parseMOL (  
    APOLparm * thee,  
    Vio * sock )
```

Definition at line 268 of file [apolparm.c](#).

9.16.2.8 APOLparm_parsePRESS()

```
VPRIVATE Vrc_Codes APOLparm_parsePRESS (  
    APOLparm * thee,  
    Vio * sock )
```

Definition at line 558 of file [apolparm.c](#).

9.16.2.9 APOLparm_parseSDENS()

```
VPRIVATE Vrc_Codes APOLparm_parseSDENS (  
    APOLparm * thee,  
    Vio * sock )
```

Definition at line 510 of file [apolparm.c](#).

9.16.2.10 APOLparm_parseSRAD()

```
VPRIVATE Vrc_Codes APOLparm_parseSRAD (  
    APOLparm * thee,  
    Vio * sock )
```

Definition at line 309 of file [apolparm.c](#).

9.16.2.11 APOLparm_parseSRFM()

```
VPRIVATE Vrc_Codes APOLparm_parseSRFM (  
    APOLparm * thee,  
    Vio * sock )
```

Definition at line 287 of file [apolparm.c](#).

9.16.2.12 APOLparm_parseSWIN()

```
VPRIVATE Vrc_Codes APOLparm_parseSWIN (  
    APOLparm * thee,  
    Vio * sock )
```

Definition at line 328 of file [apolparm.c](#).

9.16.2.13 APOLparm_parseTEMP()

```
VPRIVATE Vrc_Codes APOLparm_parseTEMP (  
    APOLparm * thee,  
    Vio * sock )
```

Definition at line 347 of file [apolparm.c](#).

9.17 apolparm.c

[Go to the documentation of this file.](#)

```

00001
00057 #include "apolparm.h"
00058
00059 VEMBED(rcsid="$Id$")
00060
00061 #if !defined(VINLINE_MGPARM)
00062
00063 #endif /* if !defined(VINLINE_MGPARM) */
00064
00065 VPUBLIC APOLparm* APOLparm_ctor() {
00066
00067     /* Set up the structure */
00068     APOLparm *thee = VNULL;
00069     thee = (APOLparm*)Vmem_malloc(VNULL, 1, sizeof(APOLparm));
00070     VASSERT( thee != VNULL);
00071     VASSERT( APOLparm_ctor2(thee) == VRC_SUCCESS );
00072
00073     return thee;
00074 }
00075
00076 VPUBLIC Vrc_Codes APOLparm_ctor2(APOLparm *thee) {
00077
00078     int i;
00079
00080     if (thee == VNULL) return VRC_FAILURE;
00081
00082     thee->parsed = 0;
00083
00084     thee->setgrid = 0;
00085     thee->setmolid = 0;
00086     thee->setbconc = 0;
00087     thee->setsdens = 0;
00088     thee->setdpos = 0;
00089     thee->setpress = 0;
00090     thee->setsrfm = 0;
00091     thee->setsrad = 0;
00092     thee->setswin = 0;
00093
00094     thee->settemp = 0;
00095     thee->setgamma = 0;
00096
00097     thee->setwat = 0;
00098
00099     thee->sav = 0.0;
00100     thee->sasa = 0.0;
00101     thee->wcaEnergy = 0.0;
00102
00103     for(i=0;i<3;i++) thee->totForce[i] = 0.0;
00104
00105     return VRC_SUCCESS;
00106 }
00107
00108 VPUBLIC void APOLparm_copy(
00109     APOLparm *thee,
00110     APOLparm *source
00111 ) {
00112
00113     int i;
00114
00115     thee->parsed = source->parsed;
00116
00117     for (i=0; i<3; i++) thee->grid[i] = source->grid[i];
00118     thee->setgrid = source->setgrid;
00119
00120     thee->molid = source->molid;
00121     thee->setmolid = source->setmolid;
00122
00123     thee->bconc = source->bconc ;
00124     thee->setbconc= source->setbconc ;
00125
00126     thee->sdens = source->sdens ;
00127     thee->setsdens= source->setsdens ;
00128
00129     thee->dpos = source->dpos ;
00130     thee->setdpos= source->setdpos ;
00131
00132     thee->press = source->press ;

```

```

00133     thee->setpress = source->setpress ;
00134
00135     thee->srfm = source->srfm ;
00136     thee->setsrfm = source->setsrfm ;
00137
00138     thee->srad = source->srad ;
00139     thee->setsrad = source->setsrad ;
00140
00141     thee->swin = source->swin ;
00142     thee->setswin = source->setswin ;
00143
00144     thee->temp = source->temp ;
00145     thee->settemp = source->settemp ;
00146
00147     thee->gamma = source->gamma ;
00148     thee->setgamma = source->setgamma ;
00149
00150     thee->calcenergy = source->calcenergy ;
00151     thee->setcalcenergy = source->setcalcenergy ;
00152
00153     thee->calcforce = source->calcforce ;
00154     thee->setcalcforce = source->setcalcforce ;
00155
00156     thee->setwat = source->setwat ;
00157
00158     thee->sav = source->sav;
00159     thee->sasa = source->sasa;
00160     thee->wcaEnergy = source->wcaEnergy;
00161
00162     for(i=0;i<3;i++) thee->totForce[i] = source->totForce[i];
00163
00164     return;
00165 }
00166
00167 VPUBLIC void APOLparm_dtor(APOLparm **thee) {
00168     if ((*thee) != VNULL) {
00169         APOLparm_dtor2(*thee);
00170         Vmem_free(VNULL, 1, sizeof(APOLparm), (void **)thee);
00171         (*thee) = VNULL;
00172     }
00173
00174     return;
00175 }
00176
00177 VPUBLIC void APOLparm_dtor2(APOLparm *thee) { ; }
00178
00179 VPUBLIC Vrc_Codes APOLparm_check(APOLparm *thee) {
00180
00181     Vrc_Codes rc;
00182     rc = VRC_SUCCESS;
00183
00184     if (!thee->parsed) {
00185         Vnm_print(2, "APOLparm_check: not filled!\n");
00186         return VRC_FAILURE;
00187     }
00188     if (!thee->setgrid) {
00189         Vnm_print(2, "APOLparm_check: grid not set!\n");
00190         rc = VRC_FAILURE;
00191     }
00192     if (!thee->setmolid) {
00193         Vnm_print(2, "APOLparm_check: molid not set!\n");
00194         rc = VRC_FAILURE;
00195     }
00196     if (!thee->setbconc) {
00197         Vnm_print(2, "APOLparm_check: bconc not set!\n");
00198         rc = VRC_FAILURE;
00199     }
00200     if (!thee->setsdens) {
00201         Vnm_print(2, "APOLparm_check: sdens not set!\n");
00202         rc = VRC_FAILURE;
00203     }
00204     if (!thee->setdpos) {
00205         Vnm_print(2, "APOLparm_check: dpos not set!\n");
00206         rc = VRC_FAILURE;
00207     }
00208     if (!thee->setpress) {
00209         Vnm_print(2, "APOLparm_check: press not set!\n");
00210         rc = VRC_FAILURE;
00211     }
00212     if (!thee->setsrfm) {

```

```

00214     Vnm_print(2, "APOLparm_check:  srfm not set!\n");
00215     rc = VRC_FAILURE;
00216 }
00217 if (!thee->setsrad) {
00218     Vnm_print(2, "APOLparm_check:  srad not set!\n");
00219     rc = VRC_FAILURE;
00220 }
00221 if (!thee->setswin) {
00222     Vnm_print(2, "APOLparm_check:  swin not set!\n");
00223     rc = VRC_FAILURE;
00224 }
00225 if (!thee->settemp) {
00226     Vnm_print(2, "APOLparm_check:  temp not set!\n");
00227     rc = VRC_FAILURE;
00228 }
00229 if (!thee->setgamma) {
00230     Vnm_print(2, "APOLparm_check:  gamma not set!\n");
00231     rc = VRC_FAILURE;
00232 }
00233 return rc;
00234 }
00235 }
00236
00237 VPRIVATE Vrc_Codes APOLparm_parseGRID(APOLparm *thee, Vio *sock) {
00238     char tok[VMAX_BUFSIZE];
00239     double tf;
00240
00241     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00242     if (sscanf(tok, "%lf", &tf) == 0) {
00243         Vnm_print(2, "Nosh:  Read non-float (%s) while parsing GRID \
00244 keyword!\n", tok);
00245         return VRC_WARNING;
00246     } else thee->grid[0] = tf;
00247     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00248     if (sscanf(tok, "%lf", &tf) == 0) {
00249         Vnm_print(2, "Nosh:  Read non-float (%s) while parsing GRID \
00250 keyword!\n", tok);
00251         return VRC_WARNING;
00252     } else thee->grid[1] = tf;
00253     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00254     if (sscanf(tok, "%lf", &tf) == 0) {
00255         Vnm_print(2, "Nosh:  Read non-float (%s) while parsing GRID \
00256 keyword!\n", tok);
00257         return VRC_WARNING;
00258     } else thee->grid[2] = tf;
00259     thee->setgrid = 1;
00260     return VRC_SUCCESS;
00261 }
00262
00263 VERROR1:
00264     Vnm_print(2, "parseAPOL:  ran out of tokens!\n");
00265     return VRC_WARNING;
00266 }
00267
00268 VPRIVATE Vrc_Codes APOLparm_parseMOL(APOLparm *thee, Vio *sock) {
00269     int ti;
00270     char tok[VMAX_BUFSIZE];
00271
00272     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00273     if (sscanf(tok, "%d", &ti) == 0) {
00274         Vnm_print(2, "Nosh:  Read non-int (%s) while parsing MOL \
00275 keyword!\n", tok);
00276         return VRC_WARNING;
00277     }
00278     thee->molid = ti;
00279     thee->setmolid = 1;
00280     return VRC_SUCCESS;
00281 }
00282 VERROR1:
00283     Vnm_print(2, "parseAPOL:  ran out of tokens!\n");
00284     return VRC_WARNING;
00285 }
00286
00287 VPRIVATE Vrc_Codes APOLparm_parseSRFM(APOLparm *thee, Vio *sock) {
00288     char tok[VMAX_BUFSIZE];
00289
00290     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00291
00292     if (Vstring_strcasecmp(tok, "sacc") == 0) {
00293         thee->srfm = VSM_MOL;
00294         thee->setsrfm = 1;

```

```

00295         return VRC_SUCCESS;
00296     } else {
00297         Vnm_print(2, "parseAPOL: Unrecongized keyword (%s) when parsing srfm!\n", tok);
00298         Vnm_print(2, "parseAPOL: Accepted values for srfm = sacc\n");
00299         return VRC_WARNING;
00300     }
00301
00302     return VRC_FAILURE;
00303
00304 ERROR1:
00305     Vnm_print(2, "parseAPOL: ran out of tokens!\n");
00306     return VRC_WARNING;
00307 }
00308
00309 VPRIVATE Vrc_Codes APOLparm_parseSRAD(APOLparm *thee, Vio *sock) {
00310     char tok[VMAX_BUFSIZE];
00311     double tf;
00312
00313     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00314     if (sscanf(tok, "%lf", &tf) == 0) {
00315         Vnm_print(2, "Nosh: Read non-float (%s) while parsing SRAD \
00316 keyword!\n", tok);
00317         return VRC_WARNING;
00318     }
00319     thee->srad = tf;
00320     thee->setsrad = 1;
00321     return VRC_SUCCESS;
00322
00323 ERROR1:
00324     Vnm_print(2, "parseAPOL: ran out of tokens!\n");
00325     return VRC_WARNING;
00326 }
00327
00328 VPRIVATE Vrc_Codes APOLparm_parseSWIN(APOLparm *thee, Vio *sock) {
00329     char tok[VMAX_BUFSIZE];
00330     double tf;
00331
00332     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00333     if (sscanf(tok, "%lf", &tf) == 0) {
00334         Vnm_print(2, "Nosh: Read non-float (%s) while parsing SWIN \
00335 keyword!\n", tok);
00336         return VRC_WARNING;
00337     }
00338     thee->swin = tf;
00339     thee->setswin = 1;
00340     return VRC_SUCCESS;
00341
00342 ERROR1:
00343     Vnm_print(2, "parseAPOL: ran out of tokens!\n");
00344     return VRC_WARNING;
00345 }
00346
00347 VPRIVATE Vrc_Codes APOLparm_parseTEMP(APOLparm *thee, Vio *sock) {
00348     char tok[VMAX_BUFSIZE];
00349     double tf;
00350
00351     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00352     if (sscanf(tok, "%lf", &tf) == 0) {
00353         Vnm_print(2, "Nosh: Read non-float (%s) while parsing TEMP \
00354 keyword!\n", tok);
00355         return VRC_WARNING;
00356     }
00357     thee->temp = tf;
00358     thee->settemp = 1;
00359     return VRC_SUCCESS;
00360
00361 ERROR1:
00362     Vnm_print(2, "parseAPOL: ran out of tokens!\n");
00363     return VRC_WARNING;
00364 }
00365
00366 VPRIVATE Vrc_Codes APOLparm_parseGAMMA(APOLparm *thee, Vio *sock) {
00367     char tok[VMAX_BUFSIZE];
00368     double tf;
00369
00370     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00371     if (sscanf(tok, "%lf", &tf) == 0) {
00372         Vnm_print(2, "Nosh: Read non-float (%s) while parsing GAMMA \
00373 keyword!\n", tok);
00374         return VRC_WARNING;
00375     }

```

```

00376     thee->gamma = tf;
00377     thee->setgamma = 1;
00378     return VRC_SUCCESS;
00379
00380 VERROR1:
00381     Vnm_print(2, "parseAPOL: ran out of tokens!\n");
00382     return VRC_WARNING;
00383 }
00384
00385 VPRIVATE Vrc_Codes APOLparm_parseCALCENERGY(APOLparm *thee, Vio *sock) {
00386     char tok[VMAX_BUFSIZE];
00387     int ti;
00388
00389     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00390     /* Parse number */
00391     if (sscanf(tok, "%d", &ti) == 1) {
00392         thee->calcenergy = (APOLparm_calcEnergy)ti;
00393         thee->setcalcenergy = 1;
00394
00395         Vnm_print(2, "parseAPOL: Warning -- parsed deprecated \"calcenergy \"
00396 %d\" statement.\n", ti);
00397         Vnm_print(2, "parseAPOL: Please use \"calcenergy \"");
00398         switch (thee->calcenergy) {
00399             case ACE_NO:
00400                 Vnm_print(2, "no");
00401                 break;
00402             case ACE_TOTAL:
00403                 Vnm_print(2, "total");
00404                 break;
00405             case ACE_COMPS:
00406                 Vnm_print(2, "comps");
00407                 break;
00408             default:
00409                 Vnm_print(2, "UNKNOWN");
00410                 break;
00411         }
00412         Vnm_print(2, "\" instead.\n");
00413         return VRC_SUCCESS;
00414     } else if (Vstring_strcasecmp(tok, "no") == 0) {
00415         thee->calcenergy = ACE_NO;
00416         thee->setcalcenergy = 1;
00417         return VRC_SUCCESS;
00418     } else if (Vstring_strcasecmp(tok, "total") == 0) {
00419         thee->calcenergy = ACE_TOTAL;
00420         thee->setcalcenergy = 1;
00421         return VRC_SUCCESS;
00422     } else if (Vstring_strcasecmp(tok, "comps") == 0) {
00423         thee->calcenergy = ACE_COMPS;
00424         thee->setcalcenergy = 1;
00425         return VRC_SUCCESS;
00426     } else {
00427         Vnm_print(2, "Nosh: Unrecognized parameter (%s) while parsing \"
00428 calcenergy!\n", tok);
00429         return VRC_WARNING;
00430     }
00431     return VRC_FAILURE;
00432
00433 VERROR1:
00434     Vnm_print(2, "parseAPOL: ran out of tokens!\n");
00435     return VRC_WARNING;
00436 }
00437
00438 VPRIVATE Vrc_Codes APOLparm_parseCALCFORCE(APOLparm *thee, Vio *sock) {
00439     char tok[VMAX_BUFSIZE];
00440     int ti;
00441
00442     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00443     /* Parse number */
00444     if (sscanf(tok, "%d", &ti) == 1) {
00445         thee->calcforce = (APOLparm_calcForce)ti;
00446         thee->setcalcforce = 1;
00447
00448         Vnm_print(2, "parseAPOL: Warning -- parsed deprecated \"calcforce \"
00449 %d\" statement.\n", ti);
00450         Vnm_print(2, "parseAPOL: Please use \"calcforce \"");
00451         switch (thee->calcenergy) {
00452             case ACF_NO:
00453                 Vnm_print(2, "no");
00454                 break;
00455             case ACF_TOTAL:
00456                 Vnm_print(2, "total");

```

```

00457         break;
00458     case ACF_COMPS:
00459         Vnm_print(2, "comps");
00460         break;
00461     default:
00462         Vnm_print(2, "UNKNOWN");
00463         break;
00464     }
00465     Vnm_print(2, "\"" instead.\n");
00466     return VRC_SUCCESS;
00467 } else if (Vstring_strcasecmp(tok, "no") == 0) {
00468     thee->calcforce = ACF_NO;
00469     thee->setcalcforce = 1;
00470     return VRC_SUCCESS;
00471 } else if (Vstring_strcasecmp(tok, "total") == 0) {
00472     thee->calcforce = ACF_TOTAL;
00473     thee->setcalcforce = 1;
00474     return VRC_SUCCESS;
00475 } else if (Vstring_strcasecmp(tok, "comps") == 0) {
00476     thee->calcforce = ACF_COMPS;
00477     thee->setcalcforce = 1;
00478     return VRC_SUCCESS;
00479 } else {
00480     Vnm_print(2, "Nosh: Unrecognized parameter (%s) while parsing \
00481 calcforce!\n", tok);
00482     return VRC_WARNING;
00483 }
00484 return VRC_FAILURE;
00485
00486 ERROR1:
00487     Vnm_print(2, "parseAPOL: ran out of tokens!\n");
00488     return VRC_WARNING;
00489 }
00490
00491 VPRIVATE Vrc_Codes APOLparm_parseBCONC(APOLparm *thee, Vio *sock) {
00492     char tok[VMAX_BUFSIZE];
00493     double tf;
00494
00495     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00496     if (sscanf(tok, "%lf", &tf) == 0) {
00497         Vnm_print(2, "Nosh: Read non-float (%s) while parsing BCONC \
00498 keyword!\n", tok);
00499         return VRC_WARNING;
00500     }
00501     thee->bconc = tf;
00502     thee->setbconc = 1;
00503     return VRC_SUCCESS;
00504
00505 ERROR1:
00506     Vnm_print(2, "parseAPOL: ran out of tokens!\n");
00507     return VRC_WARNING;
00508 }
00509
00510 VPRIVATE Vrc_Codes APOLparm_parseSDENS(APOLparm *thee, Vio *sock) {
00511     char tok[VMAX_BUFSIZE];
00512     double tf;
00513
00514     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00515     if (sscanf(tok, "%lf", &tf) == 0) {
00516         Vnm_print(2, "Nosh: Read non-float (%s) while parsing SDENS \
00517 keyword!\n", tok);
00518         return VRC_WARNING;
00519     }
00520     thee->sdens = tf;
00521     thee->setsdens = 1;
00522     return VRC_SUCCESS;
00523
00524 ERROR1:
00525     Vnm_print(2, "parseAPOL: ran out of tokens!\n");
00526     return VRC_WARNING;
00527 }
00528
00529 VPRIVATE Vrc_Codes APOLparm_parseDPOS(APOLparm *thee, Vio *sock) {
00530     char tok[VMAX_BUFSIZE];
00531     double tf;
00532
00533     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00534     if (sscanf(tok, "%lf", &tf) == 0) {
00535         Vnm_print(2, "Nosh: Read non-float (%s) while parsing SDENS \
00536 keyword!\n", tok);
00537         return VRC_WARNING;

```



```

00538     }
00539     thee->dpos = tf;
00540     thee->setdpos = 1;
00541
00542     if(thee->dpos < 0.001){
00543         Vnm_print(1, "\nWARNING WARNING WARNING WARNING\n");
00544         Vnm_print(1, "Nosh: dpos is set to a very small value.\n");
00545         Vnm_print(1, "Nosh: If you are not using a PQR file, you can \
00546 safely ignore this message.\n");
00547         Vnm_print(1, "Nosh: Otherwise please choose a value greater than \
00548 or equal to 0.001.\n\n");
00549     }
00550
00551     return VRC_SUCCESS;
00552
00553 ERROR1:
00554     Vnm_print(2, "parseAPOL: ran out of tokens!\n");
00555     return VRC_WARNING;
00556 }
00557
00558 VPRIVATE Vrc_Codes APOLparm_parsePRESS(APOLparm *thee, Vio *sock) {
00559     char tok[VMAX_BUFSIZE];
00560     double tf;
00561
00562     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00563     if (sscanf(tok, "%lf", &tf) == 0) {
00564         Vnm_print(2, "Nosh: Read non-float (%s) while parsing PRESS \
00565 keyword!\n", tok);
00566         return VRC_WARNING;
00567     }
00568     thee->press = tf;
00569     thee->setpress = 1;
00570     return VRC_SUCCESS;
00571
00572 ERROR1:
00573     Vnm_print(2, "parseAPOL: ran out of tokens!\n");
00574     return VRC_WARNING;
00575 }
00576
00577 VPUBLIC Vrc_Codes APOLparm_parseToken(APOLparm *thee, char tok[VMAX_BUFSIZE],
00578     Vio *sock) {
00579
00580     if (thee == VNULL) {
00581         Vnm_print(2, "parseAPOL: got NULL thee!\n");
00582         return VRC_WARNING;
00583     }
00584
00585     if (sock == VNULL) {
00586         Vnm_print(2, "parseAPOL: got NULL socket!\n");
00587         return VRC_WARNING;
00588     }
00589
00590     if (Vstring_strcasecmp(tok, "mol") == 0) {
00591         return APOLparm_parseMOL(thee, sock);
00592     } else if (Vstring_strcasecmp(tok, "grid") == 0) {
00593         return APOLparm_parseGRID(thee, sock);
00594     } else if (Vstring_strcasecmp(tok, "dime") == 0) {
00595         Vnm_print(2, "APOLparm_parseToken: The DIME and GLEN keywords for APOLAR have been replaced with
00596 GRID.\n");
00597         Vnm_print(2, "APOLparm_parseToken: Please see the APBS User Guide for more information.\n");
00598         return VRC_WARNING;
00599     } else if (Vstring_strcasecmp(tok, "glen") == 0) {
00600         Vnm_print(2, "APOLparm_parseToken: The DIME and GLEN keywords for APOLAR have been replaced with
00601 GRID.\n");
00602         Vnm_print(2, "APOLparm_parseToken: Please see the APBS User Guide for more information.\n");
00603         return VRC_WARNING;
00604     } else if (Vstring_strcasecmp(tok, "bconc") == 0) {
00605         return APOLparm_parseBCONC(thee, sock);
00606     } else if (Vstring_strcasecmp(tok, "sdens") == 0) {
00607         return APOLparm_parseSDENS(thee, sock);
00608     } else if (Vstring_strcasecmp(tok, "dpos") == 0) {
00609         return APOLparm_parseDPOS(thee, sock);
00610     } else if (Vstring_strcasecmp(tok, "srfm") == 0) {
00611         return APOLparm_parseSRFM(thee, sock);
00612     } else if (Vstring_strcasecmp(tok, "srad") == 0) {
00613         return APOLparm_parseSRAD(thee, sock);
00614     } else if (Vstring_strcasecmp(tok, "swin") == 0) {
00615         return APOLparm_parseSWIN(thee, sock);
00616     } else if (Vstring_strcasecmp(tok, "temp") == 0) {
00617         return APOLparm_parseTEMP(thee, sock);
00618     } else if (Vstring_strcasecmp(tok, "gamma") == 0) {

```

```

00617         return APOLparm_parseGAMMA(thee, sock);
00618     } else if (Vstring_strcasecmp(tok, "press") == 0) {
00619         return APOLparm_parsePRESS(thee, sock);
00620     } else if (Vstring_strcasecmp(tok, "calcenergy") == 0) {
00621         return APOLparm_parseCALCENERGY(thee, sock);
00622     } else if (Vstring_strcasecmp(tok, "calcforce") == 0) {
00623         return APOLparm_parseCALCFORCE(thee, sock);
00624     }
00625
00626     return VRC_FAILURE;
00627 }
00628 }

```

9.18 apolparm.h

```

00001
00063 #ifndef _APOLPARAM_H_
00064 #define _APOLPARAM_H_
00065
00066 /* Generic header files */
00067 #include "apbscfg.h"
00068
00069 #include "malloc/malloc.h"
00070
00071 #include "generic/vhal.h"
00072 #include "generic/vstring.h"
00073 #include "generic/vparam.h"
00074
00079 enum eAPOLparm_calcEnergy {
00080     ACE_NO=0,
00081     ACE_TOTAL=1,
00082     ACE_COMPS=2
00083 };
00084
00089 typedef enum eAPOLparm_calcEnergy APOLparm_calcEnergy;
00090
00095 enum eAPOLparm_calcForce {
00096     ACF_NO=0,
00097     ACF_TOTAL=1,
00098     ACF_COMPS=2
00099 };
00100
00105 typedef enum eAPOLparm_calcForce APOLparm_calcForce;
00106
00111 enum eAPOLparm_doCalc {
00112     ACD_NO=0,
00113     ACD_YES=1,
00114     ACD_ERROR=2
00115 };
00116
00121 typedef enum eAPOLparm_doCalc APOLparm_doCalc;
00122
00123
00129 struct sAPOLparm {
00130
00131     int parsed;
00133     double grid[3];
00134     int setgrid;
00136     int molid;
00137     int setmolid;
00139     double bconc;
00140     int setbconc;
00142     double sdens;
00143     int setsdens;
00145     double dpos;
00146     int setdpos;
00148     double press;
00149     int setpress;
00151     Vsurf_Meth srfm;
00152     int setsrfm;
00154     double srad;
00155     int setsrad;
00157     double swin;
00158     int setswin;
00160     double temp;
00161     int settemp;
00163     double gamma;
00165     int setgamma;

```

```

00167     APOLparm_calcEnergy calcenergy;
00168     int setcalcenergy;
00170     APOLparm_calcForce calcforce;
00171     int setcalcforce;
00173     double watsigma;
00174     double watepsilon;
00175     double sasa;
00176     double sav;
00177     double wcaEnergy;
00178     double totForce[3];
00180     int setwat;
00182 };
00183
00188 typedef struct sAPOLparm APOLparm;
00189
00190 /* ////////////////////////////////////////
00191 // Class Nosh: Non-inlineable methods (nosh.c)
00193
00199 VEXTERNC APOLparm* APOLparm_ctor();
00200
00207 VEXTERNC Vrc_Codes APOLparm_ctor2(APOLparm *thee);
00208
00214 VEXTERNC void APOLparm_dtor(APOLparm **thee);
00215
00221 VEXTERNC void APOLparm_dtor2(APOLparm *thee);
00222
00230 VEXTERNC Vrc_Codes APOLparm_check(APOLparm *thee);
00231
00238 VEXTERNC void APOLparm_copy(APOLparm *thee, APOLparm *source);
00239
00250 VEXTERNC Vrc_Codes APOLparm_parseToken(APOLparm *thee, char tok[VMAX_BUFSIZE],
00251     Vio *sock);
00252
00253 #endif
00254

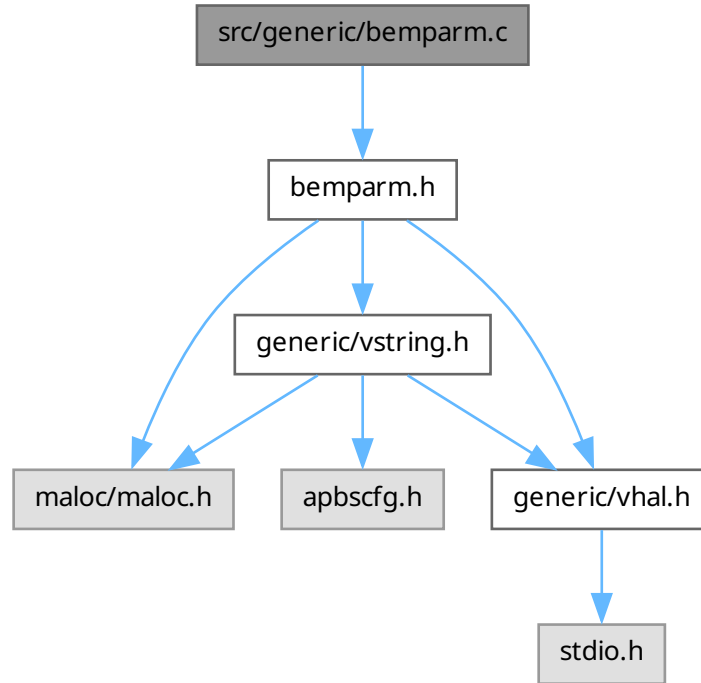
```

9.19 src/generic/bemparm.c File Reference

Class BEMparm methods.

```
#include "bemparm.h"
```

Include dependency graph for bemparm.c:



Functions

- `VPUBLIC BEMparm * BEMparm_ctor (BEMparm_CalcType type)`
Construct BEMparm object.
- `VPUBLIC Vrc_Codes BEMparm_ctor2 (BEMparm *thee, BEMparm_CalcType type)`
FORTTRAN stub to construct BEMparm object.
- `VPUBLIC void BEMparm_dtor (BEMparm **thee)`
Object destructor.
- `VPUBLIC void BEMparm_dtor2 (BEMparm *thee)`
FORTTRAN stub for object destructor.
- `VPUBLIC Vrc_Codes BEMparm_check (BEMparm *thee)`
Consistency check for parameter values stored in object.
- `VPUBLIC void BEMparm_copy (BEMparm *thee, BEMparm *parm)`
Copy object info into thee.
- `VPRIVATE Vrc_Codes BEMparm_parseTREE_ORDER (BEMparm *thee, Vio *sock)`
- `VPRIVATE Vrc_Codes BEMparm_parseTREE_N0 (BEMparm *thee, Vio *sock)`
- `VPRIVATE Vrc_Codes BEMparm_parseMAC (BEMparm *thee, Vio *sock)`
- `VPRIVATE Vrc_Codes BEMparm_parseMESH (BEMparm *thee, Vio *sock)`
- `VPRIVATE Vrc_Codes BEMparm_parseOUTDATA (BEMparm *thee, Vio *sock)`

- VPUBLIC Vrc_Codes [BEMparm_parseToken](#) ([BEMparm](#) *thee, char tok[VMAX_BUFSIZE], Vio *sock)
Parse an MG keyword from an input file.

9.19.1 Detailed Description

Class BEMparm methods.

Author

Nathan A. Baker, Weihua Geng, and Andrew J. Stevens

Version

\$Id\$

Attention

```
*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
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*   Pacific Northwest National Laboratory
*
*   Additional contributing authors listed in the code documentation.
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*   * THE POSSIBILITY OF SUCH DAMAGE.
*
*
*
```

Definition in file [bemparm.c](#).

9.19.2 Function Documentation

9.19.2.1 BEMparm_copy()

```
VPUBLIC void BEMparm_copy (
    BEMparm * thee,
    BEMparm * parm )
```

Copy object info into thee.

Author

Nathan Baker

Parameters

<i>thee</i>	destination object
<i>parm</i>	source object

Definition at line 174 of file [bemparm.c](#).

9.19.2.2 BEMparm_parseMAC()

```
VPRIVATE Vrc_Codes BEMparm_parseMAC (
    BEMparm * thee,
    Vio * sock )
```

Definition at line 256 of file [bemparm.c](#).

9.19.2.3 BEMparm_parseMESH()

```
VPRIVATE Vrc_Codes BEMparm_parseMESH (
    BEMparm * thee,
    Vio * sock )
```

Definition at line 279 of file [bemparm.c](#).

9.19.2.4 BEMparm_parseOUTDATA()

```
VPRIVATE Vrc_Codes BEMparm_parseOUTDATA (
    BEMparm * thee,
    Vio * sock )
```

Definition at line 308 of file [bemparm.c](#).

9.19.2.5 BEMparm_parseTREE_N0()

```
VPRIVATE Vrc_Codes BEMparm_parseTREE_N0 (
    BEMparm * thee,
    Vio * sock )
```

Definition at line 233 of file [bemparm.c](#).

9.19.2.6 BEMparm_parseTREE_ORDER()

```
VPRIVATE Vrc_Codes BEMparm_parseTREE_ORDER (
    BEMparm * thee,
    Vio * sock )
```

Definition at line 210 of file [bemparm.c](#).

9.20 bemparm.c

[Go to the documentation of this file.](#)

```

00001
00057 #include "bemparm.h"
00058
00059 VEMBED(rcsid="$Id$")
00060
00061 #if !defined(VINLINE_MGPARM)
00062
00063 #endif /* if !defined(VINLINE_MGPARM) */
00064
00065
00066 VPUBLIC BEMParm* BEMParm_ctor(BEMParm_CalcType type) {
00067
00068     /* Set up the structure */
00069     BEMParm *thee = VNULL;
00070     thee = (BEMParm*)Vmem_malloc(VNULL, 1, sizeof(BEMParm));
00071     VASSERT( thee != VNULL);
00072     VASSERT( BEMParm_ctor2(thee, type) == VRC_SUCCESS );
00073
00074     return thee;
00075 }
00076
00077 VPUBLIC Vrc_Codes BEMParm_ctor2(BEMParm *thee, BEMParm_CalcType type) {
00078
00079     int i;
00080
00081     if (thee == VNULL) return VRC_FAILURE;
00082
00083     thee->parsed = 0;
00084     thee->type = type;
00085
00086     /* *** GENERIC PARAMETERS *** */
00087
00088     /* *** TYPE 0 PARAMETERS *** */
00089     thee->tree_order = 1;
00090     thee->settree_order = 0;
00091     thee->tree_n0 = 500;
00092     thee->settree_n0 = 0;
00093     thee->mac = 0.8;
00094     thee->setmac = 0;
00095
00096     thee->mesh = 0;
00097     thee->setmesh = 0;
00098
00099     thee->outdata = 0;
00100     thee->setoutdata = 0;
00101
00102     /* *** TYPE 1 & 2 PARAMETERS *** */
00103
00104     /* *** TYPE 2 PARAMETERS *** */
00105     thee->nonlintype = 0;
00106     thee->setnonlintype = 0;
00107
00108     /* *** Default parameters for TINKER *** */
00109     thee->chgs = VCM_CHARGE;
00110
00111     return VRC_SUCCESS;
00112 }
00113
00114 VPUBLIC void BEMParm_dtor(BEMParm **thee) {
00115     if ((*thee) != VNULL) {
00116         BEMParm_dtor2(*thee);
00117         Vmem_free(VNULL, 1, sizeof(BEMParm), (void **)thee);
00118         (*thee) = VNULL;
00119     }
00120 }
00121
00122 VPUBLIC void BEMParm_dtor2(BEMParm *thee) { ; }
00123
00124 VPUBLIC Vrc_Codes BEMParm_check(BEMParm *thee) {
00125
00126     Vrc_Codes rc;
00127     int i, tdime[3], ti, tnlev[3], nlev;
00128
00129     rc = VRC_SUCCESS;
00130
00131     Vnm_print(0, "BEMParm_check:  checking BEMParm object of type %d.\n",
00132               thee->type);

```

```

00133
00134     /* Check to see if we were even filled... */
00135     if (!thee->parsed) {
00136         Vnm_print(2, "BEMparm_check: not filled!\n");
00137         return VRC_FAILURE;
00138     }
00139
00140
00141     /* Check type settings */
00142     if ((thee->type != BCT_MANUAL) && (thee->type != BCT_NONE)) {
00143         Vnm_print(2, "BEMparm_check: type not set");
00144         rc = VRC_FAILURE;
00145     }
00146
00147     /* Check treecode setting */
00148     if (thee->tree_order < 1) {
00149         Vnm_print(2, "BEMparm_check: treecode order is less than 1");
00150         rc = VRC_FAILURE;
00151     }
00152     if (thee->tree_n0 < 1) {
00153         Vnm_print(2, "BEMparm_check: treecode leaf size is less than 1");
00154         rc = VRC_FAILURE;
00155     }
00156     if (thee->mac > 1 || thee->mac <= 0) {
00157         Vnm_print(2, "BEMparm_check: MAC criterion fails");
00158         rc = VRC_FAILURE;
00159     }
00160
00161     if (thee->mesh > 2 || thee->mesh < 0) {
00162         Vnm_print(2, "BEMparm_check: mesh must be 0 (msms) or 1 and 2 (NanoShaper)");
00163         rc = VRC_FAILURE;
00164     }
00165
00166     if (thee->outdata > 2 || thee->outdata < 0) {
00167         Vnm_print(2, "BEMparm_check: outdata must be 0, 1 (vtk), or 2 (not specified)");
00168         rc = VRC_FAILURE;
00169     }
00170
00171     return rc;
00172 }
00173
00174 VPUBLIC void BEMparm_copy(BEMparm *thee, BEMparm *parm) {
00175
00176     int i;
00177
00178     VASSERT(thee != VNULL);
00179     VASSERT(parm != VNULL);
00180
00181
00182     thee->type = parm->type;
00183     thee->parsed = parm->parsed;
00184
00185     /* *** GENERIC PARAMETERS *** */
00186
00187     /* *** TYPE 0 PARMS *** */
00188
00189     thee->tree_order = parm->tree_order;
00190     thee->settree_order = parm->settree_order;
00191     thee->tree_n0 = parm->tree_n0;
00192     thee->settree_n0 = parm->settree_n0;
00193     thee->mac = parm->mac;
00194     thee->setmac = parm->setmac;
00195
00196     thee->mesh = parm->mesh;
00197     thee->setmesh = parm->setmesh;
00198
00199     thee->outdata = parm->outdata;
00200     thee->setoutdata = parm->setoutdata;
00201
00202     /* *** TYPE 1 & 2 PARMS *** */
00203
00204     /* *** TYPE 2 PARMS *** */
00205     thee->nonlintype = parm->nonlintype;
00206     thee->setnonlintype = parm->setnonlintype;
00207 }
00208
00209
00210 VPRIVATE Vrc_Codes BEMparm_parseTREE_ORDER(BEMparm *thee, Vio *sock) {
00211
00212     char tok[VMAX_BUFSIZE];
00213     int ti;

```



```

00214
00215     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00216     if (sscanf(tok, "%d", &ti) == 0) {
00217         Vnm_print(2, "Nosh: Read non-integer (%s) while parsing TREE_ORDER \
00218 keyword!\n", tok);
00219         return VRC_WARNING;
00220     } else if (ti <= 0) {
00221         Vnm_print(2, "parseBEM: tree_order must be greater than 0!\n");
00222         return VRC_WARNING;
00223     } else thee->tree_order = ti;
00224     thee->settree_order = 1;
00225     return VRC_SUCCESS;
00226
00227     ERROR1:
00228     Vnm_print(2, "parseBEM: ran out of tokens!\n");
00229     return VRC_WARNING;
00230 }
00231
00232
00233 VPRIVATE Vrc_Codes BEMparm_parseTREE_N0(BEMparm *thee, Vio *sock) {
00234
00235     char tok[VMAX_BUFSIZE];
00236     int ti;
00237
00238     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00239     if (sscanf(tok, "%d", &ti) == 0) {
00240         Vnm_print(2, "Nosh: Read non-integer (%s) while parsing TREE_N0 \
00241 keyword!\n", tok);
00242         return VRC_WARNING;
00243     } else if (ti <= 0) {
00244         Vnm_print(2, "parseBEM: tree_n0 must be greater than 0!\n");
00245         return VRC_WARNING;
00246     } else thee->tree_n0 = ti;
00247     thee->settree_n0 = 1;
00248     return VRC_SUCCESS;
00249
00250     ERROR1:
00251     Vnm_print(2, "parseBEM: ran out of tokens!\n");
00252     return VRC_WARNING;
00253 }
00254
00255
00256 VPRIVATE Vrc_Codes BEMparm_parseMAC(BEMparm *thee, Vio *sock) {
00257
00258     char tok[VMAX_BUFSIZE];
00259     double tf;
00260
00261     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00262     if (sscanf(tok, "%lf", &tf) == 0) {
00263         Vnm_print(2, "Nosh: Read non-float (%s) while parsing mac \
00264 keyword!\n", tok);
00265         return VRC_WARNING;
00266     } else if (tf <= 0.0 || tf > 1.0) {
00267         Vnm_print(2, "parseBEM: mac must be between 0 and 1!\n");
00268         return VRC_WARNING;
00269     } else thee->mac = tf;
00270     thee->setmac = 1;
00271     return VRC_SUCCESS;
00272
00273     ERROR1:
00274     Vnm_print(2, "parseBEM: ran out of tokens!\n");
00275     return VRC_WARNING;
00276 }
00277
00278
00279 VPRIVATE Vrc_Codes BEMparm_parseMESH(BEMparm *thee, Vio *sock) {
00280
00281     char tok[VMAX_BUFSIZE];
00282
00283     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00284     if (strcmp(tok, "msms") == 0){
00285         thee->mesh = 0;
00286     }
00287     else if (strcmp(tok, "ses") == 0){
00288         thee->mesh = 1;
00289     }
00290     else if (strcmp(tok, "skin") == 0){
00291         thee->mesh = 2;
00292     }
00293     else{
00294         Vnm_print(2, "parseBEM: mesh option %s is not recognized! It must be one of msms, \

```

```

00295         ses, or skin.\n", tok);
00296     return VRC_WARNING;
00297 }
00298
00299 thee->setmesh = 1;
00300 return VRC_SUCCESS;
00301
00302 ERROR1:
00303     Vnm_print(2, "parseBEM: ran out of tokens!\n");
00304     return VRC_WARNING;
00305 }
00306
00307
00308 VPRIVATE Vrc_Codes BEMparm_parseOUTDATA(BEMparm *thee, Vio *sock) {
00309
00310     char tok[VMAX_BUFSIZE];
00311     int ti;
00312
00313     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00314     if (sscanf(tok, "%d", &ti) == 0) {
00315         Vnm_print(2, "Nosh: Read non-integer (%s) while parsing OUTDATA \
00316             keyword!\n", tok);
00317         return VRC_WARNING;
00318     } else if (ti < 0 || ti > 2) {
00319         Vnm_print(2, "parseBEM: outdata must be 0, 1 (vtk), \
00320             or 2 (unspecified)!\n");
00321         return VRC_WARNING;
00322     } else thee->outdata = ti;
00323     thee->setoutdata = 1;
00324     return VRC_SUCCESS;
00325
00326     ERROR1:
00327         Vnm_print(2, "parseBEM: ran out of tokens!\n");
00328         return VRC_WARNING;
00329 }
00330
00331
00332 VPUBLIC Vrc_Codes BEMparm_parseToken(BEMparm *thee, char tok[VMAX_BUFSIZE],
00333     Vio *sock) {
00334
00335     if (thee == VNULL) {
00336         Vnm_print(2, "parseBEM: got NULL thee!\n");
00337         return VRC_WARNING;
00338     }
00339     if (sock == VNULL) {
00340         Vnm_print(2, "parseBEM: got NULL socket!\n");
00341         return VRC_WARNING;
00342     }
00343
00344     Vnm_print(0, "BEMparm_parseToken: trying %s...\n", tok);
00345
00346
00347     if (Vstring_strcasecmp(tok, "tree_order") == 0) {
00348         return BEMparm_parseTREE_ORDER(thee, sock);
00349     } else if (Vstring_strcasecmp(tok, "tree_n0") == 0) {
00350         return BEMparm_parseTREE_N0(thee, sock);
00351     } else if (Vstring_strcasecmp(tok, "mac") == 0) {
00352         return BEMparm_parseMAC(thee, sock);
00353     } else if (Vstring_strcasecmp(tok, "mesh") == 0) {
00354         return BEMparm_parseMESH(thee, sock);
00355     } else if (Vstring_strcasecmp(tok, "outdata") == 0) {
00356         return BEMparm_parseOUTDATA(thee, sock);
00357     } else {
00358         Vnm_print(2, "parseBEM: Unrecognized keyword (%s)!\n", tok);
00359         return VRC_WARNING;
00360     }
00361
00362     return VRC_FAILURE;
00363 }
00364 }

```

9.21 bemparm.h

```

00001
00064 #ifndef _BEMPARM_H_
00065 #define _BEMPARM_H_
00066
00067 /* Generic header files */

```

```

00068 #include "malloc/malloc.h"
00069
00070 #include "generic/vhal.h"
00071 #include "generic/vstring.h"
00072
00077 enum eBEMparm_CalcType {
00078     BCT_MANUAL=0,
00079     BCT_NONE=1
00080 };
00081
00086 typedef enum eBEMparm_CalcType BEMparm_CalcType;
00087
00096 typedef struct sBEMparm {
00097
00098     BEMparm_CalcType type;
00099     int parsed;
00101     /* *** GENERIC PARAMETERS *** */
00102     Vchrg_Src chgs;
00104     int tree_order;
00105     int settree_order;
00106     int tree_n0;
00107     int settree_n0;
00108     double mac;
00109     int setmac;
00110     int nonlintype;
00111     int setnonlintype;
00113     int mesh;
00114     int setmesh;
00116     int outdata;
00117     int setoutdata;
00119 } BEMparm;
00120
00127 VEXTERNC BEMparm* BEMparm_ctor(BEMparm_CalcType type);
00128
00136 VEXTERNC Vrc_Codes BEMparm_ctor2(BEMparm *thee, BEMparm_CalcType type);
00137
00143 VEXTERNC void BEMparm_dtor(BEMparm **thee);
00144
00150 VEXTERNC void BEMparm_dtor2(BEMparm *thee);
00151
00158 VEXTERNC Vrc_Codes BEMparm_check(BEMparm *thee);
00159
00166 VEXTERNC void BEMparm_copy(BEMparm *thee, BEMparm *parm);
00167
00177 VEXTERNC Vrc_Codes BEMparm_parseToken(BEMparm *thee, char tok[VMAX_BUFSIZE],
00178     Vio *sock);
00179
00180 #endif

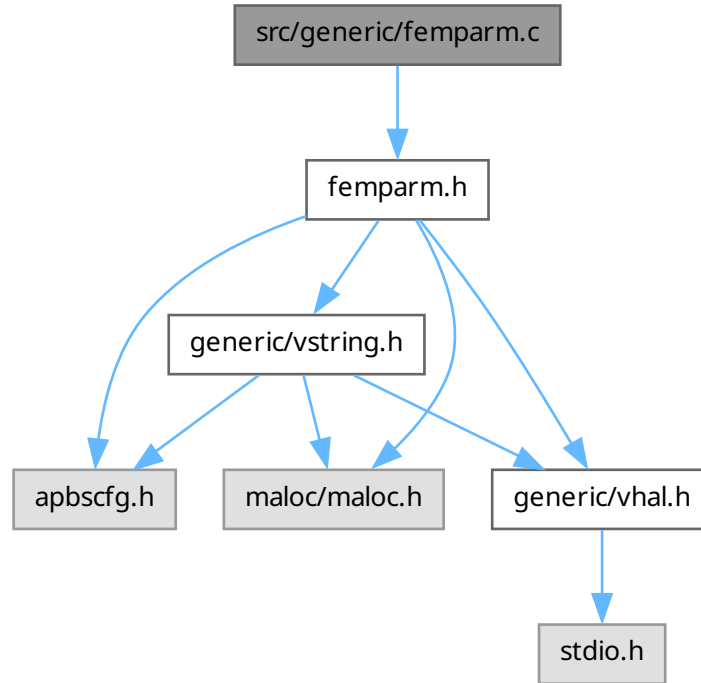
```

9.22 src/generic/femparm.c File Reference

Class FEMparm methods.

```
#include "femparm.h"
```

Include dependency graph for femparm.c:



Functions

- `VPUBLIC FEMparm * FEMparm_ctor (FEMparm_CalcType type)`
Construct FEMparm.
- `VPUBLIC int FEMparm_ctor2 (FEMparm *thee, FEMparm_CalcType type)`
FORTTRAN stub to construct FEMparm.
- `VPUBLIC void FEMparm_copy (FEMparm *thee, FEMparm *source)`
Copy target object into thee.
- `VPUBLIC void FEMparm_dtor (FEMparm **thee)`
Object destructor.
- `VPUBLIC void FEMparm_dtor2 (FEMparm *thee)`
FORTTRAN stub for object destructor.
- `VPUBLIC int FEMparm_check (FEMparm *thee)`
Consistency check for parameter values stored in object.
- `VPRIVATE Vrc_Codes FEMparm_parseDOMAINLENGTH (FEMparm *thee, Vio *sock)`
- `VPRIVATE Vrc_Codes FEMparm_parseETOL (FEMparm *thee, Vio *sock)`
- `VPRIVATE Vrc_Codes FEMparm_parseEKEY (FEMparm *thee, Vio *sock)`
- `VPRIVATE Vrc_Codes FEMparm_parseAKEYPRE (FEMparm *thee, Vio *sock)`
- `VPRIVATE Vrc_Codes FEMparm_parseAKEYSOLVE (FEMparm *thee, Vio *sock)`

- VPRIVATE Vrc_Codes [FEMparm_parseTARGETNUM](#) (FEMparm *thee, Vio *sock)
- VPRIVATE Vrc_Codes [FEMparm_parseTARGETRES](#) (FEMparm *thee, Vio *sock)
- VPRIVATE Vrc_Codes [FEMparm_parseMAXSOLVE](#) (FEMparm *thee, Vio *sock)
- VPRIVATE Vrc_Codes [FEMparm_parseMAXVERT](#) (FEMparm *thee, Vio *sock)
- VPRIVATE Vrc_Codes [FEMparm_parseUSEMESH](#) (FEMparm *thee, Vio *sock)
- VPUBLIC Vrc_Codes [FEMparm_parseToken](#) (FEMparm *thee, char tok[VMAX_BUFSIZE], Vio *sock)

Parse an MG keyword from an input file.

9.22.1 Detailed Description

Class FEMparm methods.

Author

Nathan Baker

Version

\$Id\$

Attention

```
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*
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```

```

* ARISING IN ANY WAY OUT OF THE USE OF THIS SOFTWARE, EVEN IF ADVISED OF
* THE POSSIBILITY OF SUCH DAMAGE.
*
*

```

Definition in file [femparm.c](#).

9.22.2 Function Documentation

9.22.2.1 FEMparm_parseAKEYPRE()

```

VPRIVATE Vrc_Codes FEMparm_parseAKEYPRE (
    FEMparm * thee,
    Vio * sock )

```

Definition at line 276 of file [femparm.c](#).

9.22.2.2 FEMparm_parseAKEYSOLVE()

```

VPRIVATE Vrc_Codes FEMparm_parseAKEYSOLVE (
    FEMparm * thee,
    Vio * sock )

```

Definition at line 303 of file [femparm.c](#).

9.22.2.3 FEMparm_parseDOMAINLENGTH()

```

VPRIVATE Vrc_Codes FEMparm_parseDOMAINLENGTH (
    FEMparm * thee,
    Vio * sock )

```

Definition at line 196 of file [femparm.c](#).

9.22.2.4 FEMparm_parseEKEY()

```

VPRIVATE Vrc_Codes FEMparm_parseEKEY (
    FEMparm * thee,
    Vio * sock )

```

Definition at line 244 of file [femparm.c](#).

9.22.2.5 FEMparm_parseETOL()

```

VPRIVATE Vrc_Codes FEMparm_parseETOL (
    FEMparm * thee,
    Vio * sock )

```

Definition at line 221 of file [femparm.c](#).

9.22.2.6 FEMparm_parseMAXSOLVE()

```

VPRIVATE Vrc_Codes FEMparm_parseMAXSOLVE (
    FEMparm * thee,
    Vio * sock )

```

Definition at line 372 of file [femparm.c](#).

9.22.2.7 FEMparm_parseMAXVERT()

```

VPRIVATE Vrc_Codes FEMparm_parseMAXVERT (
    FEMparm * thee,
    Vio * sock )

```

Definition at line 391 of file [femparm.c](#).

9.22.2.8 FEMparm_parseTARGETNUM()

```
VPRIVATE Vrc_Codes FEMparm_parseTARGETNUM (
    FEMparm * thee,
    Vio * sock )
```

Definition at line 333 of file [femparm.c](#).

9.22.2.9 FEMparm_parseTARGETRES()

```
VPRIVATE Vrc_Codes FEMparm_parseTARGETRES (
    FEMparm * thee,
    Vio * sock )
```

Definition at line 352 of file [femparm.c](#).

9.22.2.10 FEMparm_parseUSEMESH()

```
VPRIVATE Vrc_Codes FEMparm_parseUSEMESH (
    FEMparm * thee,
    Vio * sock )
```

Definition at line 411 of file [femparm.c](#).

9.23 femparm.c

[Go to the documentation of this file.](#)

```
00001
00057 #include "femparm.h"
00058
00059 VEMBED(rcsid="$Id$")
00060
00061 #if !defined(VINLINE_MGPARM)
00062
00063 #endif /* if !defined(VINLINE_MGPARM) */
00064
00065 VPUBLIC FEMparm* FEMparm_ctor(FEMparm_CalcType type) {
00066
00067     /* Set up the structure */
00068     FEMparm *thee = VNULL;
00069     thee = (FEMparm*)Vmem_malloc(VNULL, 1, sizeof(FEMparm));
00070     VASSERT( thee != VNULL);
00071     VASSERT( FEMparm_ctor2(thee, type) );
00072
00073     return thee;
00074 }
00075
00076 VPUBLIC int FEMparm_ctor2(FEMparm *thee,
00077                         FEMparm_CalcType type
00078                         ) {
00079
00080     if (thee == VNULL) return 0;
00081
00082     thee->parsed = 0;
00083     thee->type = type;
00084     thee->settype = 1;
00085
00086     thee->setglen = 0;
00087     thee->setetol = 0;
00088     thee->setekey = 0;
00089     thee->setakeyPRE = 0;
00090     thee->setakeySOLVE = 0;
00091     thee->settargetNum = 0;
00092     thee->settargetRes = 0;
00093     thee->setmaxsolve = 0;
00094     thee->setmaxvert = 0;
00095     thee->useMesh = 0;
00096
00097     return 1;
00098 }
00099
00100 VPUBLIC void FEMparm_copy(
```

```

00101             FEMparm *thee,
00102             FEMparm *source
00103         ) {
00104
00105         int i;
00106
00107         thee->parsed = source->parsed;
00108         thee->type = source->type;
00109         thee->settype = source->settype;
00110         for (i=0; i<3; i++) thee->glen[i] = source->glen[i];
00111         thee->setglen = source->setglen;
00112         thee->etol = source->etol;
00113         thee->setetol = source->setetol;
00114         thee->ekey = source->ekey;
00115         thee->setekey = source->setekey;
00116         thee->akeyPRE = source->akeyPRE;
00117         thee->setakeyPRE = source->setakeyPRE;
00118         thee->akeySOLVE = source->akeySOLVE;
00119         thee->setakeySOLVE = source->setakeySOLVE;
00120         thee->targetNum = source->targetNum;
00121         thee->settargetNum = source->settargetNum;
00122         thee->targetRes = source->targetRes;
00123         thee->settargetRes = source->settargetRes;
00124         thee->maxsolve = source->maxsolve;
00125         thee->setmaxsolve = source->setmaxsolve;
00126         thee->maxvert = source->maxvert;
00127         thee->setmaxvert = source->setmaxvert;
00128         thee->pkey = source->pkey;
00129         thee->useMesh = source->useMesh;
00130         thee->meshID = source->meshID;
00131     }
00132
00133 VPUBLIC void FEMparm_dtor(FEMparm **thee) {
00134     if ((*thee) != VNULL) {
00135         FEMparm_dtor2(*thee);
00136         Vmem_free(VNULL, 1, sizeof(FEMparm), (void **)thee);
00137         (*thee) = VNULL;
00138     }
00139 }
00140
00141 VPUBLIC void FEMparm_dtor2(FEMparm *thee) { ; }
00142
00143 VPUBLIC int FEMparm_check(FEMparm *thee) {
00144     int rc;
00145     rc = 1;
00146
00147     if (!thee->parsed) {
00148         Vnm_print(2, "FEMparm_check: not filled!\n");
00149         return 0;
00150     }
00151     if (!thee->settype) {
00152         Vnm_print(2, "FEMparm_check: type not set!\n");
00153         rc = 0;
00154     }
00155     if (!thee->setglen) {
00156         Vnm_print(2, "FEMparm_check: glen not set!\n");
00157         rc = 0;
00158     }
00159     if (!thee->setetol) {
00160         Vnm_print(2, "FEMparm_check: etol not set!\n");
00161         rc = 0;
00162     }
00163     if (!thee->setekey) {
00164         Vnm_print(2, "FEMparm_check: ekey not set!\n");
00165         rc = 0;
00166     }
00167     if (!thee->setakeyPRE) {
00168         Vnm_print(2, "FEMparm_check: akeyPRE not set!\n");
00169         rc = 0;
00170     }
00171     if (!thee->setakeySOLVE) {
00172         Vnm_print(2, "FEMparm_check: akeySOLVE not set!\n");
00173         rc = 0;
00174     }
00175     if (!thee->settargetNum) {
00176         Vnm_print(2, "FEMparm_check: targetNum not set!\n");
00177         rc = 0;
00178     }
00179     if (!thee->settargetRes) {
00180         Vnm_print(2, "FEMparm_check: targetRes not set!\n");
00181     }

```



```

00182         rc = 0;
00183     }
00184     if (!thee->setmaxsolve) {
00185         Vnm_print(2, "FEMparm_check: maxsolve not set!\n");
00186         rc = 0;
00187     }
00188     if (!thee->setmaxvert) {
00189         Vnm_print(2, "FEMparm_check: maxvert not set!\n");
00190         rc = 0;
00191     }
00192 }
00193 return rc;
00194 }
00195
00196 VPRIVATE Vrc_Codes FEMparm_parseDOMAINLENGTH(FEMparm *thee,
00197                                               Vio *sock
00198                                               ) {
00199
00200     int i;
00201     double tf;
00202     char tok[VMAX_BUFSIZE];
00203
00204     for (i=0; i<3; i++) {
00205         VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00206         if (sscanf(tok, "%lf", &tf) == 0) {
00207             Vnm_print(2, "parseFE: Read non-double (%s) while parsing \
00208 DOMAINLENGTH keyword!\n", tok);
00209             return VRC_FAILURE;
00210         }
00211         thee->glen[i] = tf;
00212     }
00213     thee->setglen = 1;
00214     return VRC_SUCCESS;
00215 ERROR1:
00216     Vnm_print(2, "parseFE: ran out of tokens!\n");
00217     return VRC_FAILURE;
00218 }
00219 }
00220
00221 VPRIVATE Vrc_Codes FEMparm_parseETOL(FEMparm *thee,
00222                                       Vio *sock
00223                                       ) {
00224
00225     double tf;
00226     char tok[VMAX_BUFSIZE];
00227
00228     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00229     if (sscanf(tok, "%lf", &tf) == 0) {
00230         Vnm_print(2, "parseFE: Read non-double (%s) while parsing \
00231 ETOL keyword!\n", tok);
00232         return VRC_FAILURE;
00233     }
00234     thee->etol = tf;
00235     thee->setetol = 1;
00236     return VRC_SUCCESS;
00237 ERROR1:
00238     Vnm_print(2, "parseFE: ran out of tokens!\n");
00239     return VRC_FAILURE;
00240 }
00241 }
00242 }
00243
00244 VPRIVATE Vrc_Codes FEMparm_parseEKEY(FEMparm *thee,
00245                                       Vio *sock
00246                                       ) {
00247
00248     char tok[VMAX_BUFSIZE];
00249     Vrc_Codes vrc = VRC_FAILURE;
00250
00251     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00252     if (Vstring_strcasecmp(tok, "simp") == 0) {
00253         thee->ekey = FET_SIMP;
00254         thee->setekey = 1;
00255         vrc = VRC_SUCCESS;
00256     } else if (Vstring_strcasecmp(tok, "glob") == 0) {
00257         thee->ekey = FET_GLOB;
00258         thee->setekey = 1;
00259         vrc = VRC_SUCCESS;
00260     } else if (Vstring_strcasecmp(tok, "frac") == 0) {
00261         thee->ekey = FET_FRAC;
00262         thee->setekey = 1;

```

```

00263         vrc = VRC_SUCCESS;
00264     } else {
00265         Vnm_print(2, "parseFE: undefined value (%s) for ekey!\n", tok);
00266         vrc = VRC_FAILURE;
00267     }
00268
00269     return vrc;
00270 ERROR1:
00271     Vnm_print(2, "parseFE: ran out of tokens!\n");
00272     return VRC_FAILURE;
00273 }
00274 }
00275
00276 VPRIVATE Vrc_Codes FEMparm_parseAKEYPRE(FEMparm *thee, Vio *sock) {
00277
00278     char tok[VMAX_BUFSIZE];
00279     Vrc_Codes vrc = VRC_FAILURE;
00280
00281     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00282     if (Vstring_strcasecmp(tok, "unif") == 0) {
00283         thee->akeyPRE = FRT_UNIF;
00284         thee->setakeyPRE = 1;
00285         vrc = VRC_SUCCESS;
00286     } else if (Vstring_strcasecmp(tok, "geom") == 0) {
00287         thee->akeyPRE = FRT_GEOM;
00288         thee->setakeyPRE = 1;
00289         vrc = VRC_SUCCESS;
00290     } else {
00291         Vnm_print(2, "parseFE: undefined value (%s) for akeyPRE!\n", tok);
00292         vrc = VRC_FAILURE;
00293     }
00294
00295     return vrc;
00296
00297 ERROR1:
00298     Vnm_print(2, "parseFE: ran out of tokens!\n");
00299     return VRC_FAILURE;
00300 }
00301 }
00302
00303 VPRIVATE Vrc_Codes FEMparm_parseAKEYSOLVE(FEMparm *thee, Vio *sock) {
00304
00305     char tok[VMAX_BUFSIZE];
00306     Vrc_Codes vrc = VRC_FAILURE;
00307
00308     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00309     if (Vstring_strcasecmp(tok, "resi") == 0) {
00310         thee->akeySOLVE = FRT_RESI;
00311         thee->setakeySOLVE = 1;
00312         vrc = VRC_SUCCESS;
00313     } else if (Vstring_strcasecmp(tok, "dual") == 0) {
00314         thee->akeySOLVE = FRT_DUAL;
00315         thee->setakeySOLVE = 1;
00316         vrc = VRC_SUCCESS;
00317     } else if (Vstring_strcasecmp(tok, "loca") == 0) {
00318         thee->akeySOLVE = FRT_LOCA;
00319         thee->setakeySOLVE = 1;
00320         vrc = VRC_SUCCESS;
00321     } else {
00322         Vnm_print(2, "parseFE: undefined value (%s) for akeyPRE!\n", tok);
00323         vrc = VRC_FAILURE;
00324     }
00325
00326     return vrc;
00327 ERROR1:
00328     Vnm_print(2, "parseFE: ran out of tokens!\n");
00329     return VRC_SUCCESS;
00330 }
00331 }
00332
00333 VPRIVATE Vrc_Codes FEMparm_parseTARGETNUM(FEMparm *thee, Vio *sock) {
00334
00335     char tok[VMAX_BUFSIZE];
00336     int ti;
00337
00338     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00339     if (sscanf(tok, "%d", &ti) == 0) {
00340         Vnm_print(2, "parseFE: read non-int (%s) for targetNum!\n", tok);
00341         return VRC_FAILURE;
00342     }
00343     thee->targetNum = ti;

```

```

00344     thee->settargetNum = 1;
00345     return VRC_SUCCESS;
00346  ERROR1:
00347     Vnm_print(2, "parseFE: ran out of tokens!\n");
00348     return VRC_FAILURE;
00349 }
00350 }
00351
00352  VPRIVATE Vrc_Codes FEMparm_parseTARGETRES(FEMparm *thee, Vio *sock) {
00353     char tok[VMAX_BUFSIZE];
00354     double tf;
00355
00356     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00357     if (sscanf(tok, "%lf", &tf) == 0) {
00358         Vnm_print(2, "parseFE: read non-double (%s) for targetNum!\n",
00359             tok);
00360         return VRC_FAILURE;
00361     }
00362     thee->targetRes = tf;
00363     thee->settargetRes = 1;
00364     return VRC_SUCCESS;
00365  ERROR1:
00366     Vnm_print(2, "parseFE: ran out of tokens!\n");
00367     return VRC_FAILURE;
00368 }
00369 }
00370 }
00371
00372  VPRIVATE Vrc_Codes FEMparm_parseMAXSOLVE(FEMparm *thee, Vio *sock) {
00373     char tok[VMAX_BUFSIZE];
00374     int ti;
00375
00376     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00377     if (sscanf(tok, "%d", &ti) == 0) {
00378         Vnm_print(2, "parseFE: read non-int (%s) for maxsolve!\n", tok);
00379         return VRC_FAILURE;
00380     }
00381     thee->maxsolve = ti;
00382     thee->setmaxsolve = 1;
00383     return VRC_SUCCESS;
00384  ERROR1:
00385     Vnm_print(2, "parseFE: ran out of tokens!\n");
00386     return VRC_FAILURE;
00387 }
00388 }
00389 }
00390
00391  VPRIVATE Vrc_Codes FEMparm_parseMAXVERT(FEMparm *thee, Vio *sock) {
00392     char tok[VMAX_BUFSIZE];
00393     int ti;
00394
00395     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00396     if (sscanf(tok, "%d", &ti) == 0) {
00397         Vnm_print(2, "parseFE: read non-int (%s) for maxvert!\n", tok);
00398         return VRC_FAILURE;
00399     }
00400     thee->maxvert = ti;
00401     thee->setmaxvert = 1;
00402     return VRC_SUCCESS;
00403  ERROR1:
00404     Vnm_print(2, "parseFE: ran out of tokens!\n");
00405     return VRC_FAILURE;
00406 }
00407 }
00408 }
00409 }
00410
00411  VPRIVATE Vrc_Codes FEMparm_parseUSEMESH(FEMparm *thee, Vio *sock) {
00412     char tok[VMAX_BUFSIZE];
00413     int ti;
00414
00415     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00416     if (sscanf(tok, "%d", &ti) == 0) {
00417         Vnm_print(2, "parseFE: read non-int (%s) for usemesh!\n", tok);
00418         return VRC_FAILURE;
00419     }
00420     thee->useMesh = 1;
00421     thee->meshID = ti;
00422     return VRC_SUCCESS;
00423 }
00424 }

```

```

00425 ERROR1:
00426     Vnm_print(2, "parsePBE: ran out of tokens!\n");
00427     return VRC_FAILURE;
00428 }
00429
00430
00431 VPUBLIC Vrc_Codes FEMparm_parseToken(FEMparm *thee, char tok[VMAX_BUFSIZE],
00432     Vio *sock) {
00433
00434     //int i, ti; // gcc says unused
00435     //double tf; // gcc says unused
00436
00437     if (thee == VNULL) {
00438         Vnm_print(2, "parseFE: got NULL thee!\n");
00439         return VRC_FAILURE;
00440     }
00441
00442     if (sock == VNULL) {
00443         Vnm_print(2, "parseFE: got NULL socket!\n");
00444         return VRC_FAILURE;
00445     }
00446
00447     if (Vstring_strcasecmp(tok, "domainLength") == 0) {
00448         return FEMparm_parseDOMAINLENGTH(thee, sock);
00449     } else if (Vstring_strcasecmp(tok, "etol") == 0) {
00450         return FEMparm_parseETOL(thee, sock);
00451     } else if (Vstring_strcasecmp(tok, "ekey") == 0) {
00452         return FEMparm_parseEKEY(thee, sock);
00453     } else if (Vstring_strcasecmp(tok, "akeyPRE") == 0) {
00454         return FEMparm_parseAKEYPRE(thee, sock);
00455     } else if (Vstring_strcasecmp(tok, "akeySOLVE") == 0) {
00456         return FEMparm_parseAKEYSOLVE(thee, sock);
00457     } else if (Vstring_strcasecmp(tok, "targetNum") == 0) {
00458         return FEMparm_parseTARGETNUM(thee, sock);
00459     } else if (Vstring_strcasecmp(tok, "targetRes") == 0) {
00460         return FEMparm_parseTARGETRES(thee, sock);
00461     } else if (Vstring_strcasecmp(tok, "maxsolve") == 0) {
00462         return FEMparm_parseMAXSOLVE(thee, sock);
00463     } else if (Vstring_strcasecmp(tok, "maxvert") == 0) {
00464         return FEMparm_parseMAXVERT(thee, sock);
00465     } else if (Vstring_strcasecmp(tok, "usemesh") == 0) {
00466         return FEMparm_parseUSEMESH(thee, sock);
00467     }
00468
00469     return VRC_WARNING;
00470
00471 }

```

9.24 src/generic/femparm.h File Reference

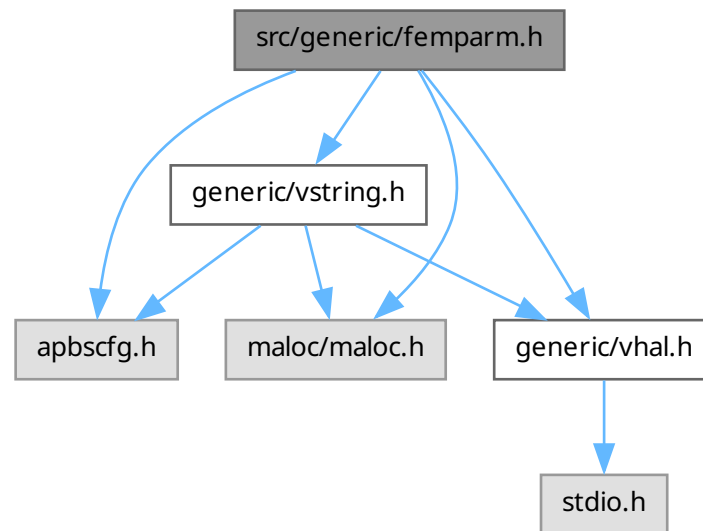
Contains declarations for class APOLparm.

```

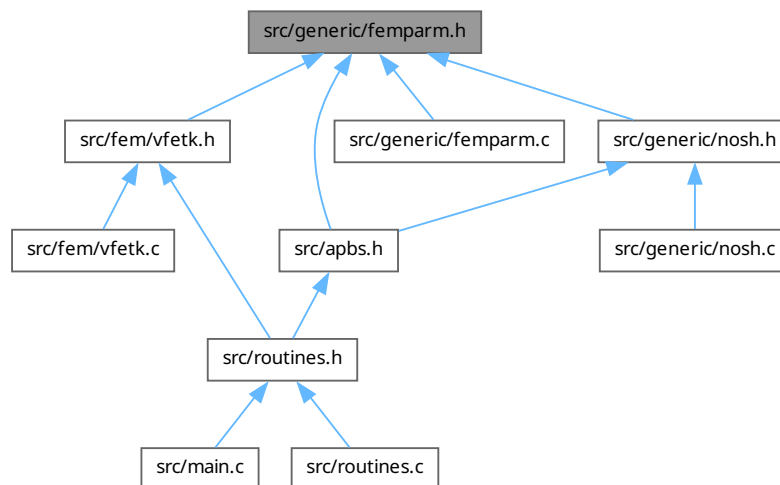
#include "apbscfg.h"
#include "malloc/malloc.h"
#include "generic/vhal.h"
#include "generic/vstring.h"

```

Include dependency graph for femparm.h:



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [sFEMparm](#)

Parameter structure for FEM-specific variables from input files.

Typedefs

- typedef enum [eFEMparm_EtolType](#) FEMparm_EtolType
Declare FEparm_EtolType type.
- typedef enum [eFEMparm_EstType](#) FEMparm_EstType
Declare FEMparm_EstType type.
- typedef enum [eFEMparm_CalcType](#) FEMparm_CalcType
Declare FEMparm_CalcType type.
- typedef struct [sFEMparm](#) FEMparm

Enumerations

- enum [eFEMparm_EtolType](#) { FET_SIMP =0 , FET_GLOB =1 , FET_FRAC =2 }
Adaptive refinement error estimate tolerance key.
- enum [eFEMparm_EstType](#) {
FRT_UNIF =0 , FRT_GEOM =1 , FRT_RESI =2 , FRT_DUAL =3 ,
FRT_LOCA =4 }
Adaptive refinement error estimator method.
- enum [eFEMparm_CalcType](#) { FCT_MANUAL , FCT_NONE }
Calculation type.

Functions

- VEXTERNC [FEMparm](#) * [FEMparm_ctor](#) ([FEMparm_CalcType](#) type)
Construct FEMparm.
- VEXTERNC int [FEMparm_ctor2](#) ([FEMparm](#) *thee, [FEMparm_CalcType](#) type)
FORTTRAN stub to construct FEMparm.
- VEXTERNC void [FEMparm_dtor](#) ([FEMparm](#) **thee)
Object destructor.
- VEXTERNC void [FEMparm_dtor2](#) ([FEMparm](#) *thee)
FORTTRAN stub for object destructor.
- VEXTERNC int [FEMparm_check](#) ([FEMparm](#) *thee)
Consistency check for parameter values stored in object.
- VEXTERNC void [FEMparm_copy](#) ([FEMparm](#) *thee, [FEMparm](#) *source)
Copy target object into thee.
- VEXTERNC Vrc_Codes [FEMparm_parseToken](#) ([FEMparm](#) *thee, char tok[VMAX_BUFSIZE], Vio *sock)
Parse an MG keyword from an input file.

9.24.1 Detailed Description

Contains declarations for class APOLparm.

Contains declarations for class FEMparm.

Version

\$Id\$

Author

Nathan A. Baker

Attention

```

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* Pacific Northwest National Laboratory
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*
*

```

Definition in file [femparm.h](#).

9.24.2 Typedef Documentation**9.24.2.1 FEMparm**

typedef struct [sFEMparm](#) [FEMparm](#)

Definition at line 182 of file [femparm.h](#).

9.25 femparm.h

[Go to the documentation of this file.](#)

```

00001
00063 #ifndef _FEMPARM_H_
00064 #define _FEMPARM_H_
00065
00066 /* Generic header files */

```

```

00067 #include "apbscfg.h"
00068
00069 #include "malloc/malloc.h"
00070
00071 #include "generic/vhal.h"
00072 #include "generic/vstring.h"
00073
00079 enum eFEMparm_EtolType {
00080     FET_SIMP=0,
00081     FET_GLOB=1,
00082     FET_FRAC=2
00083 };
00084
00090 typedef enum eFEMparm_EtolType FEMparm_EtolType;
00091
00098 enum eFEMparm_EstType {
00099     FRT_UNIF=0,
00100     FRT_GEOM=1,
00101     FRT_RESI=2,
00102     FRT_DUAL=3,
00104     FRT_LOCA=4
00105 };
00106
00111 typedef enum eFEMparm_EstType FEMparm_EstType;
00112
00117 enum eFEMparm_CalcType {
00118     FCT_MANUAL,
00119     FCT_NONE
00120 };
00121
00126 typedef enum eFEMparm_CalcType FEMparm_CalcType;
00127
00133 struct sFEMparm {
00134
00135     int parsed;
00138     FEMparm_CalcType type;
00139     int settype;
00140     double glen[3];
00141     int setglen;
00142     double etol;
00144     int setetol;
00145     FEMparm_EtolType ekey;
00147     int setekey;
00148     FEMparm_EstType akeyPRE;
00151     int setakeyPRE;
00152     FEMparm_EstType akeySOLVE;
00154     int setakeySOLVE;
00155     int targetNum;
00159     int settargetNum;
00160     double targetRes;
00164     int settargetRes;
00165     int maxsolve;
00166     int setmaxsolve;
00167     int maxvert;
00169     int setmaxvert;
00170     int pkey;
00173     int useMesh;
00174     int meshID;
00176 };
00177
00182 typedef struct sFEMparm FEMparm;
00183
00184 /* ////////////////////////////////////////
00185 // Class NOsh: Non-inlineable methods (nosh.c)
00187
00194 VEXTERNC FEMparm* FEMparm_ctor(FEMparm_CalcType type);
00195
00203 VEXTERNC int FEMparm_ctor2(FEMparm *thee, FEMparm_CalcType type);
00204
00210 VEXTERNC void FEMparm_dtor(FEMparm **thee);
00211
00217 VEXTERNC void FEMparm_dtor2(FEMparm *thee);
00218
00226 VEXTERNC int FEMparm_check(FEMparm *thee);
00227
00234 VEXTERNC void FEMparm_copy(FEMparm *thee, FEMparm *source);
00235
00246 VEXTERNC Vrc_Codes FEMparm_parseToken(FEMparm *thee, char tok[VMAX_BUFSIZE],
00247     Vio *sock);
00248
00249 #endif

```

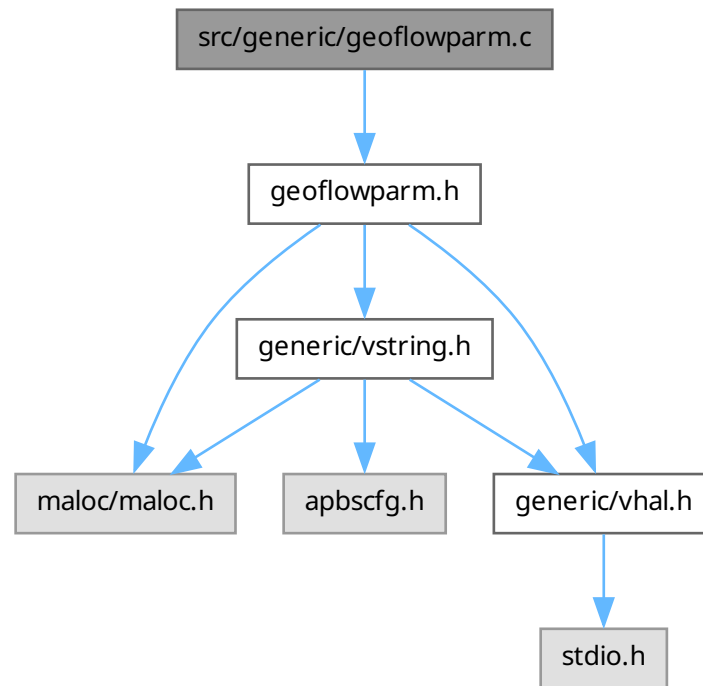

00250

9.26 src/generic/geoflowparm.c File Reference

Class GEOFLOWparm methods.

```
#include "geoflowparm.h"
```

Include dependency graph for geoflowparm.c:



Functions

- VPUBLIC [GEOFLOWparm](#) * [GEOFLOWparm_ctor](#) ([GEOFLOWparm_CalcType](#) type)
Construct GEOFLOWparm object.
- VPUBLIC Vrc_Codes [GEOFLOWparm_ctor2](#) ([GEOFLOWparm](#) *thee, [GEOFLOWparm_CalcType](#) type)
FORTTRAN stub to construct GEOFLOWparm object ??????????!!!!!!
- VPUBLIC void [GEOFLOWparm_dtor](#) ([GEOFLOWparm](#) **thee)
Object destructor.
- VPUBLIC void [GEOFLOWparm_dtor2](#) ([GEOFLOWparm](#) *thee)
FORTTRAN stub for object destructor ??????????!!!!!!
- VPUBLIC Vrc_Codes [GEOFLOWparm_check](#) ([GEOFLOWparm](#) *thee)
Consistency check for parameter values stored in object.
- VPUBLIC void [GEOFLOWparm_copy](#) ([GEOFLOWparm](#) *thee, [GEOFLOWparm](#) *parm)
copy GEOFLOWparm object int thee.

- Vrc_Codes [FUBAR](#) (const char *name)
- Vrc_Codes [parseNonNeg](#) (double *tf, double def, int *set, char *name, Vio *sock)
- VPRIVATE Vrc_Codes [GEOFLOWparm_parseVDW](#) ([GEOFLOWparm](#) *thee, Vio *sock)
- VPRIVATE Vrc_Codes [GEOFLOWparm_parseETOL](#) ([GEOFLOWparm](#) *thee, Vio *sock)
- VPUBLIC Vrc_Codes [GEOFLOWparm_parseToken](#) ([GEOFLOWparm](#) *thee, char tok[VMAX_BUFSIZE], Vio *sock)

Parse an MG keyword from an input file.

9.26.1 Detailed Description

Class GEOFLOWparm methods.

Author

Andrew Stevens

Version

\$Id\$

Attention

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*

```

Definition in file [geoflowparm.c](#).

9.26.2 Function Documentation

9.26.2.1 FUBAR()

```

Vrc_Codes FUBAR (
    const char * name )

```

Definition at line 138 of file [geoflowparm.c](#).

9.26.2.2 GEOFLOWparm_parseETOL()

```

VPRIVATE Vrc_Codes GEOFLOWparm_parseETOL (
    GEOFLOWparm * thee,
    Vio * sock )

```

Definition at line 186 of file [geoflowparm.c](#).

9.26.2.3 GEOFLOWparm_parseVDW()

```

VPRIVATE Vrc_Codes GEOFLOWparm_parseVDW (
    GEOFLOWparm * thee,
    Vio * sock )

```

Definition at line 164 of file [geoflowparm.c](#).

9.26.2.4 parseNonNeg()

```

Vrc_Codes parseNonNeg (
    double * tf,
    double def,
    int * set,
    char * name,
    Vio * sock )

```

Definition at line 143 of file [geoflowparm.c](#).

9.27 geoflowparm.c

[Go to the documentation of this file.](#)

```

00001
00057 #include "geoflowparm.h"
00058
00059 VEMBED(rcsid="$Id$")
00060
00061 #if !defined(VINLINE_MGPARM)
00062
00063 #endif /* if !defined(VINLINE_MGPARM) */
00064
00065
00066 VPUBLIC GEOFLOWparm* GEOFLOWparm_ctor(GEOFLOWparm_CalcType type) {
00067     /* Set up the structure */
00068     GEOFLOWparm *thee = VNULL;
00069     thee = (GEOFLOWparm*)Vmem_malloc(VNULL, 1, sizeof(GEOFLOWparm));
00070     VASSERT( thee != VNULL);
00071     VASSERT( GEOFLOWparm_ctor2(thee, type) == VRC_SUCCESS );
00072
00073     return thee;
00074 }
00075

```

```

00076
00077 VPUBLIC Vrc_Codes GEOFLOWparm_ctor2(GEOFLOWparm *thee, GEOFLOWparm_CalcType type) {
00078
00079     int i;
00080
00081     if (thee == VNULL) return VRC_FAILURE;
00082
00083     thee->parsed = 0;
00084     thee->type = type;
00085     thee->vdw = 0;
00086     thee->etol = 1.0e-6;
00087
00088     return VRC_SUCCESS;
00089 }
00090
00091 VPUBLIC void GEOFLOWparm_dtor(GEOFLOWparm **thee) {
00092     if ((*thee) != VNULL) {
00093         GEOFLOWparm_dtor2(*thee);
00094         Vmem_free(VNULL, 1, sizeof(GEOFLOWparm), (void **)thee);
00095         (*thee) = VNULL;
00096     }
00097 }
00098
00099 VPUBLIC void GEOFLOWparm_dtor2(GEOFLOWparm *thee) { ; }
00100
00101 VPUBLIC Vrc_Codes GEOFLOWparm_check(GEOFLOWparm *thee) {
00102
00103     Vrc_Codes rc;
00104
00105     rc = VRC_SUCCESS;
00106
00107     Vnm_print(0, "GEOFLOWparm_check: checking GEOFLOWparm object of type %d.\n",
00108             thee->type);
00109
00110     /* Check to see if we were even filled... */
00111     if (!thee->parsed) {
00112         Vnm_print(2, "GEOFLOWparm_check: not filled!\n");
00113         return VRC_FAILURE;
00114     }
00115
00116
00117     /* Check type settings */
00118     //if ((thee->type != GFCT_MANUAL)&& (thee->type != GFCT_AUTO)&& (thee->type != GFCT_NONE)) {
00119     if (thee->type != GFCT_AUTO) {
00120         Vnm_print(2, "GEOFLOWparm_check: type not set");
00121         rc = VRC_FAILURE;
00122     }
00123
00124     return rc;
00125 }
00126
00127 VPUBLIC void GEOFLOWparm_copy(GEOFLOWparm *thee, GEOFLOWparm *parm) {
00128     VASSERT(thee != VNULL);
00129     VASSERT(parm != VNULL);
00130
00131     thee->type = parm->type;
00132     thee->parsed = parm->parsed;
00133
00134     thee->vdw = parm->vdw;
00135     thee->etol = parm->etol;
00136 }
00137
00138 Vrc_Codes FUBAR(const char* name){
00139     Vnm_print(2, "parseGEOFLOW: ran out of tokens on %s!\n", name);
00140     return VRC_WARNING;
00141 }
00142
00143 Vrc_Codes parseNonNeg(double* tf, double def, int* set, char* name, Vio* sock){
00144     char tok[VMAX_BUFSIZE];
00145     if (Vio_scanf(sock, "%s", tok) == 0) {
00146         *tf = def;
00147         return FUBAR(name);
00148     }
00149
00150     if (sscanf(tok, "%lf", tf) == 0){
00151         Vnm_print(2, "Nosh: Read non-float (%s) while parsing %s keyword!\n", tok, name);
00152         *tf = def;
00153         return VRC_WARNING;
00154     }else if (*tf < 0.0){
00155         Vnm_print(2, "parseGEOFLOW: %s must be greater than 0!\n", name);
00156         *tf = def;

```

```

00157         return VRC_WARNING;
00158     }
00159
00160     *set = 1;
00161     return VRC_SUCCESS;
00162 }
00163
00164 VPRIVATE Vrc_Codes GEOFLOWparm_parseVDW(GEOFLOWparm *thee, Vio *sock){
00165     const char* name = "vdw";
00166     char tok[VMAX_BUFSIZE];
00167     int tf;
00168     if(Vio_scanf(sock, "%s", tok) == 0) {
00169         return FUBAR(name);
00170     }
00171
00172
00173     if (sscanf(tok, "%u", &tf) == 0){
00174         Vnm_print(2, "Nosh: Read non-unsigned int (%s) while parsing %s keyword!\n", tok, name);
00175         return VRC_WARNING;
00176     } else if (tf != 0 && tf != 1){
00177         Vnm_print(2, "parseGEOFLOW: %s must be 0 or 1!\n", name);
00178         return VRC_WARNING;
00179     } else {
00180         thee->vdw = tf;
00181     }
00182     thee->setvdw = 1;
00183     return VRC_SUCCESS;
00184 }
00185
00186 VPRIVATE Vrc_Codes GEOFLOWparm_parseETOL(GEOFLOWparm *thee, Vio *sock){
00187     char tok[VMAX_BUFSIZE];
00188     double tf;
00189
00190
00191     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00192     if(sscanf(tok, "%lf", &tf) == 0){
00193         Vnm_print(2, "Nosh: Read non-float (%s) while parsing etol keyword!\n", tok);
00194         return VRC_WARNING;
00195     } else if (tf <= 0.0) {
00196         Vnm_print(2, "parseGEOFLOW: etol must be greater than 0!\n");
00197         return VRC_WARNING;
00198     } else {
00199         thee->etol = tf;
00200     }
00201
00202
00203     return VRC_SUCCESS;
00204
00205
00206 VERROR1:
00207     Vnm_print(2, "parseGEOFLOW: ran out of tokens!\n");
00208     return VRC_WARNING;
00209 }
00210
00211
00212 VPUBLIC Vrc_Codes GEOFLOWparm_parseToken(GEOFLOWparm *thee, char tok[VMAX_BUFSIZE],
00213     Vio *sock) {
00214
00215     if (thee == VNULL) {
00216         Vnm_print(2, "parseGEOFLOW: got NULL thee!\n");
00217         return VRC_WARNING;
00218     }
00219     if (sock == VNULL) {
00220         Vnm_print(2, "parseGEOFLOW: got NULL socket!\n");
00221         return VRC_WARNING;
00222     }
00223
00224     Vnm_print(0, "GEOFLOWparm_parseToken: trying %s...\n", tok);
00225
00226     if (Vstring_strcasecmp(tok, "vdwdisp") == 0) {
00227         return GEOFLOWparm_parseVDW(thee, sock);
00228     } else if (Vstring_strcasecmp(tok, "etol") == 0){
00229         return GEOFLOWparm_parseETOL(thee, sock);
00230     } else {
00231         Vnm_print(2, "parseGEOFLOW: Unrecognized keyword (%s)!\n", tok);
00232         return VRC_WARNING;
00233     }
00234
00235
00236     return VRC_FAILURE;
00237 }

```

9.28 src/generic/geoflowparm.h File Reference

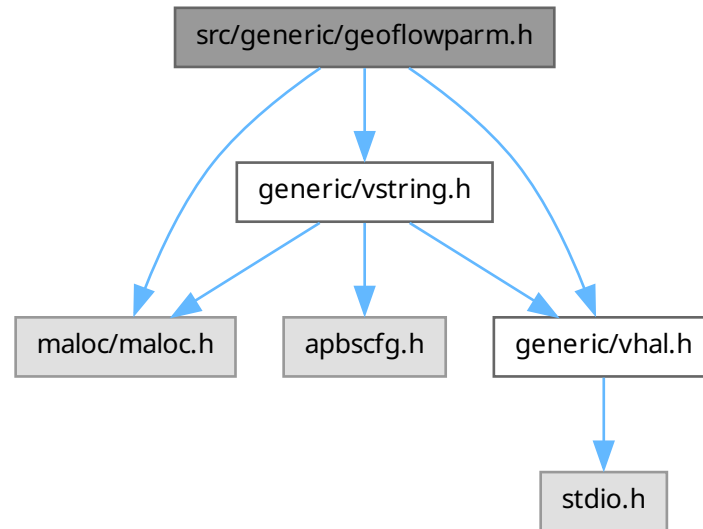
Contains declarations for class GEOFLOWparm.

```
#include "maloc/maloc.h"
```

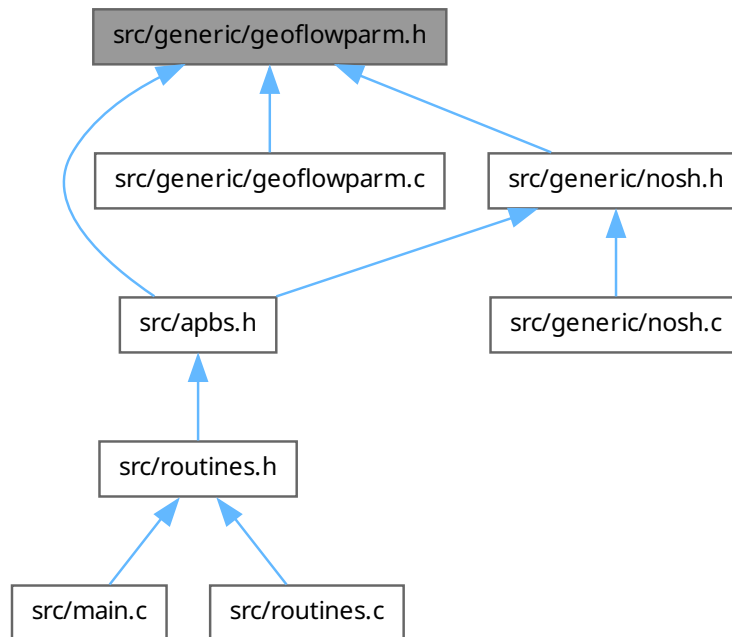
```
#include "generic/vhal.h"
```

```
#include "generic/vstring.h"
```

Include dependency graph for geoflowparm.h:



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [sGEOFLOWparm](#)
Parameter structure for GEOFLOW-specific variables from input files.

Typedefs

- typedef enum [eGEOFLOWparm_CalcType](#) [GEOFLOWparm_CalcType](#)
Declare GEOFLOWparm_CalcType type.
- typedef struct [sGEOFLOWparm](#) [GEOFLOWparm](#)
Parameter structure for GEOFLOW-specific variables from input files.

Enumerations

- enum [eGEOFLOWparm_CalcType](#) { [GFCT_AUTO](#) =1 }
Calculation type.

Functions

- VEXTERNC [GEOFLOWparm](#) * [GEOFLOWparm_ctor](#) ([GEOFLOWparm_CalcType](#) type)
Construct GEOFLOWparm object.
- VEXTERNC Vrc_Codes [GEOFLOWparm_ctor2](#) ([GEOFLOWparm](#) *thee, [GEOFLOWparm_CalcType](#) type)
FORTTRAN stub to construct GEOFLOWparm object ??????????!!!!!!

- VEXTERNC void [GEOFLOWparm_dtor](#) ([GEOFLOWparm](#) **thee)
Object destructor.
- VEXTERNC void [GEOFLOWparm_dtor2](#) ([GEOFLOWparm](#) *thee)
FORTTRAN stub for object destructor ??????????!!!!!!!
- VEXTERNC Vrc_Codes [GEOFLOWparm_check](#) ([GEOFLOWparm](#) *thee)
Consistency check for parameter values stored in object.
- VEXTERNC Vrc_Codes [GEOFLOWparm_parseToken](#) ([GEOFLOWparm](#) *thee, char tok[VMAX_BUFSIZE], Vio *sock)
Parse an MG keyword from an input file.
- VEXTERNC void [GEOFLOWparm_copy](#) ([GEOFLOWparm](#) *thee, [GEOFLOWparm](#) *parm)
copy GEOFLOWparm object into thee.
- VPRIVATE Vrc_Codes [GEOFLOWparm_parseVDW](#) ([GEOFLOWparm](#) *thee, Vio *sock)
- VPRIVATE Vrc_Codes [GEOFLOWparm_parseETOL](#) ([GEOFLOWparm](#) *thee, Vio *sock)

9.28.1 Detailed Description

Contains declarations for class [GEOFLOWparm](#).

Version

\$Id\$

Author

Andrew Stevens

Attention

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* Pacific Northwest National Laboratory
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```

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```

Definition in file [geoflowparm.h](#).

9.28.2 Function Documentation

9.28.2.1 GEOFLOWparm_parseETOL()

```

VPRIVATE Vrc_Codes GEOFLOWparm_parseETOL (
    GEOFLOWparm * thee,
    Vio * sock )

```

Definition at line 186 of file [geoflowparm.c](#).

9.28.2.2 GEOFLOWparm_parseVDW()

```

VPRIVATE Vrc_Codes GEOFLOWparm_parseVDW (
    GEOFLOWparm * thee,
    Vio * sock )

```

Definition at line 164 of file [geoflowparm.c](#).

9.29 geoflowparm.h

[Go to the documentation of this file.](#)

```

00001
00064 #ifndef _GEOFLOWPARM_H_
00065 #define _GEOFLOWPARM_H_
00066
00067 /* Generic header files */
00068 #include "malloc/malloc.h"
00069
00070 #include "generic/vhal.h"
00071 #include "generic/vstring.h"
00072
00077 enum eGEOFLOWparm_CalcType {
00078     //other methods disabled for now only auto currently implemented.
00079     //GFCT_MANUAL=0,  /**< GEOFLOW-manual */
00080     GFCT_AUTO=1,
00081     //GFCT_NONE=2 /**< not defined */
00082 };
00083
00088 typedef enum eGEOFLOWparm_CalcType GEOFLOWparm_CalcType;
00089
00098 typedef struct sGEOFLOWparm {
00099
00100     GEOFLOWparm_CalcType type;
00101     int parsed;
00103     /* *** GENERIC PARAMETERS *** */
00104     int vdw;
00105     int setvdw;
00106     double etol;
00108 } GEOFLOWparm;
00109
00116 VEXTERNC GEOFLOWparm* GEOFLOWparm_ctor(GEOFLOWparm_CalcType type);
00117
00125 VEXTERNC Vrc_Codes GEOFLOWparm_ctor2(GEOFLOWparm *thee, GEOFLOWparm_CalcType type);
00126

```

```

00132 VEXTERNC void      GEOFLOWparm_dtor(GEOFLOWparm **thee);
00133
00139 VEXTERNC void      GEOFLOWparm_dtor2(GEOFLOWparm *thee);
00140
00147 VEXTERNC Vrc_Codes GEOFLOWparm_check(GEOFLOWparm *thee);
00148
00158 VEXTERNC Vrc_Codes GEOFLOWparm_parseToken(GEOFLOWparm *thee, char tok[VMAX_BUFSIZE],
00159      Vio *sock);
00167 VEXTERNC void GEOFLOWparm_copy(GEOFLOWparm *thee, GEOFLOWparm *parm);
00168
00169 VPRIVATE Vrc_Codes GEOFLOWparm_parseVDW(GEOFLOWparm *thee, Vio *sock);
00170
00171 VPRIVATE Vrc_Codes GEOFLOWparm_parseETOL(GEOFLOWparm *thee, Vio *sock);
00172
00173
00174
00175 #endif
00176

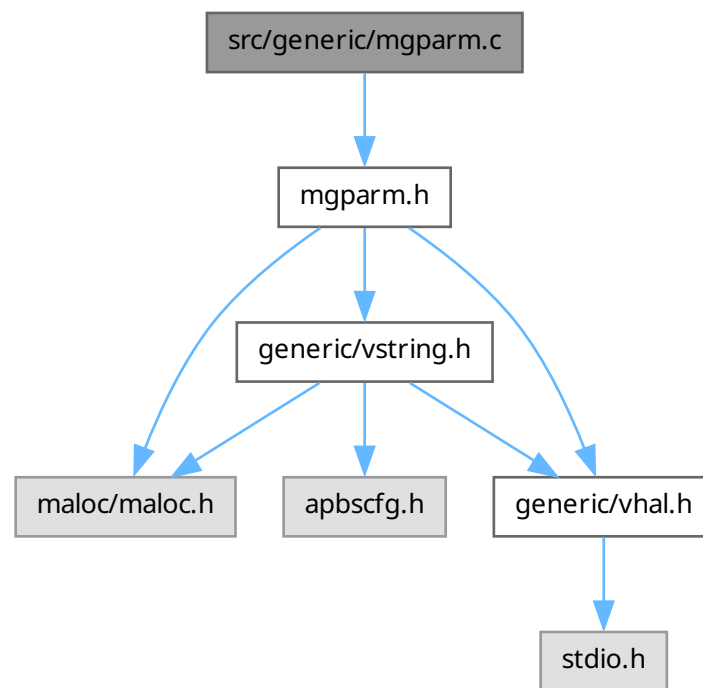
```

9.30 src/generic/mgparm.c File Reference

Class MGparm methods.

```
#include "mgparm.h"
```

Include dependency graph for mgparm.c:



Functions

- VPUBLIC void `MGparm_setCenterX` (`MGparm *thee`, double `x`)
Set center x-coordinate.

- VPUBLIC void [MGparm_setCenterY](#) ([MGparm](#) *thee, double y)
Set center y-coordinate.
- VPUBLIC void [MGparm_setCenterZ](#) ([MGparm](#) *thee, double z)
Set center z-coordinate.
- VPUBLIC double [MGparm_getCenterX](#) ([MGparm](#) *thee)
Get center x-coordinate.
- VPUBLIC double [MGparm_getCenterY](#) ([MGparm](#) *thee)
Get center y-coordinate.
- VPUBLIC double [MGparm_getCenterZ](#) ([MGparm](#) *thee)
Get center z-coordinate.
- VPUBLIC int [MGparm_getNx](#) ([MGparm](#) *thee)
Get number of grid points in x direction.
- VPUBLIC int [MGparm_getNy](#) ([MGparm](#) *thee)
Get number of grid points in y direction.
- VPUBLIC int [MGparm_getNz](#) ([MGparm](#) *thee)
Get number of grid points in z direction.
- VPUBLIC double [MGparm_getHx](#) ([MGparm](#) *thee)
Get grid spacing in x direction (Å)
- VPUBLIC double [MGparm_getHy](#) ([MGparm](#) *thee)
Get grid spacing in y direction (Å)
- VPUBLIC double [MGparm_getHz](#) ([MGparm](#) *thee)
Get grid spacing in z direction (Å)
- VPUBLIC [MGparm](#) * [MGparm_ctor](#) ([MGparm_CalcType](#) type)
Construct MGparm object.
- VPUBLIC Vrc_Codes [MGparm_ctor2](#) ([MGparm](#) *thee, [MGparm_CalcType](#) type)
FORTTRAN stub to construct MGparm object.
- VPUBLIC void [MGparm_dtor](#) ([MGparm](#) **thee)
Object destructor.
- VPUBLIC void [MGparm_dtor2](#) ([MGparm](#) *thee)
FORTTRAN stub for object destructor.
- VPUBLIC Vrc_Codes [MGparm_check](#) ([MGparm](#) *thee)
Consistency check for parameter values stored in object.
- VPUBLIC void [MGparm_copy](#) ([MGparm](#) *thee, [MGparm](#) *parm)
Copy MGparm object into thee.
- VPRIVATE Vrc_Codes [MGparm_parseDIME](#) ([MGparm](#) *thee, Vio *sock)
- VPRIVATE Vrc_Codes [MGparm_parseCHGM](#) ([MGparm](#) *thee, Vio *sock)
- VPRIVATE Vrc_Codes [MGparm_parseNLEV](#) ([MGparm](#) *thee, Vio *sock)
- VPRIVATE Vrc_Codes [MGparm_parseETOL](#) ([MGparm](#) *thee, Vio *sock)
- VPRIVATE Vrc_Codes [MGparm_parseGRID](#) ([MGparm](#) *thee, Vio *sock)
- VPRIVATE Vrc_Codes [MGparm_parseGLEN](#) ([MGparm](#) *thee, Vio *sock)
- VPRIVATE Vrc_Codes [MGparm_parseGAMMA](#) ([MGparm](#) *thee, Vio *sock)
- VPRIVATE Vrc_Codes [MGparm_parseGCENT](#) ([MGparm](#) *thee, Vio *sock)
- VPRIVATE Vrc_Codes [MGparm_parseCGLEN](#) ([MGparm](#) *thee, Vio *sock)
- VPRIVATE Vrc_Codes [MGparm_parseFGLEN](#) ([MGparm](#) *thee, Vio *sock)
- VPRIVATE Vrc_Codes [MGparm_parseCGCENT](#) ([MGparm](#) *thee, Vio *sock)
- VPRIVATE Vrc_Codes [MGparm_parseFGCENT](#) ([MGparm](#) *thee, Vio *sock)
- VPRIVATE Vrc_Codes [MGparm_parsePDIME](#) ([MGparm](#) *thee, Vio *sock)
- VPRIVATE Vrc_Codes [MGparm_parseOFRAC](#) ([MGparm](#) *thee, Vio *sock)

- VPRIVATE Vrc_Codes [MGparm_parseASYNC](#) (MGparm *thee, Vio *sock)
- VPRIVATE Vrc_Codes [MGparm_parseUSEAQUA](#) (MGparm *thee, Vio *sock)
- VPUBLIC Vrc_Codes [MGparm_parseToken](#) (MGparm *thee, char tok[VMAX_BUFSIZE], Vio *sock)

Parse an MG keyword from an input file.

9.30.1 Detailed Description

Class MGparm methods.

Author

Nathan Baker

Version

\$Id\$

Attention

```
*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
* Nathan A. Baker (nathan.baker@pnnl.gov)
* Pacific Northwest National Laboratory
*
* Additional contributing authors listed in the code documentation.
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*
*
```

Definition in file [mgparm.c](#).

9.30.2 Function Documentation

9.30.2.1 MGparm_parseASYNC()

```
VPRIVATE Vrc_Codes MGparm_parseASYNC (
    MGparm * thee,
    Vio * sock )
```

Definition at line 892 of file [mgparm.c](#).

9.30.2.2 MGparm_parseCGCENT()

```
VPRIVATE Vrc_Codes MGparm_parseCGCENT (
    MGparm * thee,
    Vio * sock )
```

Definition at line 730 of file [mgparm.c](#).

9.30.2.3 MGparm_parseCGLEN()

```
VPRIVATE Vrc_Codes MGparm_parseCGLEN (
    MGparm * thee,
    Vio * sock )
```

Definition at line 668 of file [mgparm.c](#).

9.30.2.4 MGparm_parseCHGM()

```
VPRIVATE Vrc_Codes MGparm_parseCHGM (
    MGparm * thee,
    Vio * sock )
```

Definition at line 446 of file [mgparm.c](#).

9.30.2.5 MGparm_parseDIME()

```
VPRIVATE Vrc_Codes MGparm_parseDIME (
    MGparm * thee,
    Vio * sock )
```

Definition at line 415 of file [mgparm.c](#).

9.30.2.6 MGparm_parseETOL()

```
VPRIVATE Vrc_Codes MGparm_parseETOL (
    MGparm * thee,
    Vio * sock )
```

Definition at line 516 of file [mgparm.c](#).

9.30.2.7 MGparm_parseFGCENT()

```
VPRIVATE Vrc_Codes MGparm_parseFGCENT (
    MGparm * thee,
    Vio * sock )
```

Definition at line 782 of file [mgparm.c](#).

9.30.2.8 MGparm_parseFGLEN()

```
VPRIVATE Vrc_Codes MGparm_parseFGLEN (
    MGparm * thee,
    Vio * sock )
```

Definition at line 699 of file [mgparm.c](#).

9.30.2.9 MGparm_parseGAMMA()

```
VPRIVATE Vrc_Codes MGparm_parseGAMMA (
    MGparm * thee,
    Vio * sock )
```

Definition at line 601 of file [mgparm.c](#).

9.30.2.10 MGparm_parseGCENT()

```
VPRIVATE Vrc_Codes MGparm_parseGCENT (
    MGparm * thee,
    Vio * sock )
```

Definition at line 616 of file [mgparm.c](#).

9.30.2.11 MGparm_parseGLEN()

```
VPRIVATE Vrc_Codes MGparm_parseGLEN (
    MGparm * thee,
    Vio * sock )
```

Definition at line 570 of file [mgparm.c](#).

9.30.2.12 MGparm_parseGRID()

```
VPRIVATE Vrc_Codes MGparm_parseGRID (
    MGparm * thee,
    Vio * sock )
```

Definition at line 539 of file [mgparm.c](#).

9.30.2.13 MGparm_parseNLEV()

```
VPRIVATE Vrc_Codes MGparm_parseNLEV (
    MGparm * thee,
    Vio * sock )
```

Definition at line 497 of file [mgparm.c](#).

9.30.2.14 MGparm_parseOFRAC()

```
VPRIVATE Vrc_Codes MGparm_parseOFRAC (
    MGparm * thee,
    Vio * sock )
```

Definition at line 872 of file [mgparm.c](#).

9.30.2.15 MGparm_parsePDIME()

```
VPRIVATE Vrc_Codes MGparm_parsePDIME (
    MGparm * thee,
    Vio * sock )
```

Definition at line 834 of file [mgparm.c](#).

9.30.2.16 MGparm_parseUSEAQUA()

```
VPRIVATE Vrc_Codes MGparm_parseUSEAQUA (
    MGparm * thee,
    Vio * sock )
```

Definition at line 912 of file mgparm.c.

9.31 mgparm.c

[Go to the documentation of this file.](#)

```

00001
00057 #include "mgparm.h"
00058
00059 VEMBED(rcsid="$Id$")
00060
00061 #if !defined(VINLINE_MGPARM)
00062
00063 #endif /* if !defined(VINLINE_MGPARM) */
00064
00065 VPUBLIC void MGparm_setCenterX(MGparm *thee, double x) {
00066     VASSERT(thee != VNULL);
00067     thee->center[0] = x;
00068 }
00069 VPUBLIC void MGparm_setCenterY(MGparm *thee, double y) {
00070     VASSERT(thee != VNULL);
00071     thee->center[1] = y;
00072 }
00073 VPUBLIC void MGparm_setCenterZ(MGparm *thee, double z) {
00074     VASSERT(thee != VNULL);
00075     thee->center[2] = z;
00076 }
00077 VPUBLIC double MGparm_getCenterX(MGparm *thee) {
00078     VASSERT(thee != VNULL);
00079     return thee->center[0];
00080 }
00081 VPUBLIC double MGparm_getCenterY(MGparm *thee) {
00082     VASSERT(thee != VNULL);
00083     return thee->center[1];
00084 }
00085 VPUBLIC double MGparm_getCenterZ(MGparm *thee) {
00086     VASSERT(thee != VNULL);
00087     return thee->center[2];
00088 }
00089 VPUBLIC int MGparm_getNx(MGparm *thee) {
00090     VASSERT(thee != VNULL);
00091     return thee->dime[0];
00092 }
00093 VPUBLIC int MGparm_getNy(MGparm *thee) {
00094     VASSERT(thee != VNULL);
00095     return thee->dime[1];
00096 }
00097 VPUBLIC int MGparm_getNz(MGparm *thee) {
00098     VASSERT(thee != VNULL);
00099     return thee->dime[2];
00100 }
00101 VPUBLIC double MGparm_getHx(MGparm *thee) {
00102     VASSERT(thee != VNULL);
00103     return thee->grid[0];
00104 }
00105 VPUBLIC double MGparm_getHy(MGparm *thee) {
00106     VASSERT(thee != VNULL);
00107     return thee->grid[1];
00108 }
00109 VPUBLIC double MGparm_getHz(MGparm *thee) {
00110     VASSERT(thee != VNULL);
00111     return thee->grid[2];
00112 }
00113
00114 VPUBLIC MGparm* MGparm_ctor(MGparm_CalcType type) {
00115
00116     /* Set up the structure */
00117     MGparm *thee = VNULL;
00118     thee = (MGparm*)Vmem_malloc(VNULL, 1, sizeof(MGparm));
00119     VASSERT( thee != VNULL);
00120     VASSERT( MGparm_ctor2(thee, type) == VRC_SUCCESS );
00121
00122     return thee;
00123 }
00124
00125 VPUBLIC Vrc_Codes MGparm_ctor2(MGparm *thee, MGparm_CalcType type) {
00126
00127     int i;
00128

```

```

00129     if (thee == VNULL) return VRC_FAILURE;
00130
00131     for (i=0; i<3; i++) {
00132         thee->dime[i] = -1;
00133         thee->pdime[i] = 1;
00134     }
00135
00136     thee->parsed = 0;
00137     thee->type = type;
00138
00139     /* *** GENERIC PARAMETERS *** */
00140     thee->setdime = 0;
00141     thee->setchgm = 0;
00142
00143     /* *** TYPE 0 PARAMETERS *** */
00144     thee->nlev = VMGNLEV;
00145     thee->setnlev = 1;
00146     thee->etol = 1.0e-6;
00147     thee->setetol = 0;
00148     thee->setgrid = 0;
00149     thee->setglen = 0;
00150     thee->setgcent = 0;
00151
00152     /* *** TYPE 1 & 2 PARAMETERS *** */
00153     thee->setcglen = 0;
00154     thee->setfglen = 0;
00155     thee->setcgcent = 0;
00156     thee->setfgcent = 0;
00157
00158     /* *** TYPE 2 PARAMETERS *** */
00159     thee->setpdime = 0;
00160     thee->setrank = 0;
00161     thee->setsize = 0;
00162     thee->setofrac = 0;
00163     for (i=0; i<6; i++) thee->partDisjOwnSide[i] = 0;
00164     thee->setasynch = 0;
00165
00166     /* *** Default parameters for TINKER *** */
00167     thee->chgs = VCM_CHARGE;
00168
00169     thee->useAqua = 0;
00170     thee->setUseAqua = 0;
00171
00172     return VRC_SUCCESS;
00173 }
00174
00175 VPUBLIC void MGparm_dtor(MGparm **thee) {
00176     if ((*thee) != VNULL) {
00177         MGparm_dtor2(*thee);
00178         Vmem_free(VNULL, 1, sizeof(MGparm), (void **)thee);
00179         (*thee) = VNULL;
00180     }
00181 }
00182
00183 VPUBLIC void MGparm_dtor2(MGparm *thee) { ; }
00184
00185 VPUBLIC Vrc_Codes MGparm_check(MGparm *thee) {
00186
00187     Vrc_Codes rc;
00188     int i, tdime[3], ti, tnlev[3], nlev;
00189
00190     rc = VRC_SUCCESS;
00191
00192     Vnm_print(0, "MGparm_check: checking MGparm object of type %d.\n",
00193         thee->type);
00194
00195     /* Check to see if we were even filled... */
00196     if (!thee->parsed) {
00197         Vnm_print(2, "MGparm_check: not filled!\n");
00198         return VRC_FAILURE;
00199     }
00200
00201     /* Check generic settings */
00202     if (!thee->setdime) {
00203         Vnm_print(2, "MGparm_check: DIME not set!\n");
00204         rc = VRC_FAILURE;
00205     }
00206     if (!thee->setchgm) {
00207         Vnm_print(2, "MGparm_check: CHGM not set!\n");
00208         return VRC_FAILURE;
00209     }

```



```

00210
00211
00212 /* Check sequential manual & dummy settings */
00213 if ((thee->type == MCT_MANUAL) || (thee->type == MCT_DUMMY)) {
00214     if ((!thee->setgrid) && (!thee->setglen)) {
00215         Vnm_print(2, "MGparm_check: Neither GRID nor GLEN set!\n");
00216         rc = VRC_FAILURE;
00217     }
00218     if ((thee->setgrid) && (thee->setglen)) {
00219         Vnm_print(2, "MGparm_check: Both GRID and GLEN set!\n");
00220         rc = VRC_FAILURE;
00221     }
00222     if (!thee->setgcent) {
00223         Vnm_print(2, "MGparm_check: GCENT not set!\n");
00224         rc = VRC_FAILURE;
00225     }
00226 }
00227
00228 /* Check sequential and parallel automatic focusing settings */
00229 if ((thee->type == MCT_AUTO) || (thee->type == MCT_PARALLEL)) {
00230     if (!thee->setcglen) {
00231         Vnm_print(2, "MGparm_check: CGLEN not set!\n");
00232         rc = VRC_FAILURE;
00233     }
00234     if (!thee->setfglen) {
00235         Vnm_print(2, "MGparm_check: FGLEN not set!\n");
00236         rc = VRC_FAILURE;
00237     }
00238     if (!thee->setgcent) {
00239         Vnm_print(2, "MGparm_check: CGCENT not set!\n");
00240         rc = VRC_FAILURE;
00241     }
00242     if (!thee->setfgcent) {
00243         Vnm_print(2, "MGparm_check: FGCENT not set!\n");
00244         rc = VRC_FAILURE;
00245     }
00246 }
00247
00248 /* Check parallel automatic focusing settings */
00249 if (thee->type == MCT_PARALLEL) {
00250     if (!thee->setpdime) {
00251         Vnm_print(2, "MGparm_check: PDIME not set!\n");
00252         rc = VRC_FAILURE;
00253     }
00254     if (!thee->setrank) {
00255         Vnm_print(2, "MGparm_check: PROC_RANK not set!\n");
00256         rc = VRC_FAILURE;
00257     }
00258     if (!thee->setsize) {
00259         Vnm_print(2, "MGparm_check: PROC_SIZE not set!\n");
00260         rc = VRC_FAILURE;
00261     }
00262     if (!thee->setfrac) {
00263         Vnm_print(2, "MGparm_check: OFRAC not set!\n");
00264         rc = VRC_FAILURE;
00265     }
00266 }
00267
00268 /* Perform a sanity check on nlev and dime, resetting values as necessary */
00269 if (rc == 1) {
00270     /* Calculate the actual number of grid points and nlev to satisfy the
00271      * formula:  $n = c * 2^{(l+1)} + 1$ , where  $n$  is the number of grid points,
00272      *  $c$  is an integer, and  $l$  is the number of levels */
00273     if (thee->type != MCT_DUMMY) {
00274         for (i=0; i<3; i++) {
00275             /* See if the user picked a reasonable value, if not then fix it */
00276             ti = thee->dime[i] - 1;
00277             if (ti == VPOW(2, (thee->nlev+1))) {
00278                 tnlev[i] = thee->nlev;
00279                 tdime[i] = thee->dime[i];
00280             } else {
00281                 tdime[i] = thee->dime[i];
00282                 ti = tdime[i] - 1;
00283                 tnlev[i] = 0;
00284                 /* Find the maximum number of times this dimension can be
00285                  * divided by two */
00286                 while (VEVEN(ti)) {
00287                     (tnlev[i])++;
00288                     ti = (int)ceil(0.5*ti);
00289                 }
00290                 (tnlev[i])--;

```

```

00291         /* We'd like to have at least VMGNLEV levels in the multigrid
00292         * hierarchy. This means that the dimension needs to be
00293         *  $c \cdot 2^{\text{VMGNLEV}} + 1$ , where  $c$  is an integer. */
00294         if ((tdime[i] > 65) && (tnlev[i] < VMGNLEV)) {
00295             Vnm_print(2, "Nosh: Bad dime[%d] = %d (%d nlev)!\n",
00296                 i, tdime[i], tnlev[i]);
00297             ti = (int)(tdime[i]/VPOW(2., (VMGNLEV+1)));
00298             if (ti < 1) ti = 1;
00299             tdime[i] = ti*(int)(VPOW(2., (VMGNLEV+1))) + 1;
00300             tnlev[i] = 4;
00301             Vnm_print(2, "Nosh: Reset dime[%d] to %d and (nlev = %d).\n", i, tdime[i], VMGNLEV);
00302         }
00303     }
00304 }
00305 } else { /* We are a dummy calculation, but we still need positive numbers of points */
00306     for (i=0; i<3; i++) {
00307         tnlev[i] = thee->nlev;
00308         tdime[i] = thee->dime[i];
00309         if (thee->dime[i] <= 0) {
00310             Vnm_print(2, "Nosh: Resetting dime[%d] from %d to 3.\n", i, thee->dime[i]);
00311             thee->dime[i] = 3;
00312         }
00313     }
00314 }
00315
00316 /* The actual number of levels we'll be using is the smallest number of
00317 * possible levels in any dimensions */
00318 nlev = VMIN2(tnlev[0], tnlev[1]);
00319 nlev = VMIN2(nlev, tnlev[2]);
00320 /* Set the number of levels and dimensions */
00321 Vnm_print(0, "Nosh: nlev = %d, dime = (%d, %d, %d)\n", nlev, tdime[0],
00322     tdime[1], tdime[2]);
00323 thee->nlev = nlev;
00324 if (thee->nlev <= 0) {
00325     Vnm_print(2, "MGparm_check: illegal nlev (%d); check your grid dimensions!\n", thee->nlev);
00326     rc = VRC_FAILURE;
00327 }
00328 if (thee->nlev < 2) {
00329     Vnm_print(2, "MGparm_check: you're using a very small nlev (%d) and therefore\n",
thee->nlev);
00330     Vnm_print(2, "MGparm_check: will not get the optimal performance of the multigrid\n");
00331     Vnm_print(2, "MGparm_check: algorithm. Please check your grid dimensions.\n");
00332 }
00333 for (i=0; i<3; i++) thee->dime[i] = tdime[i];
00334 }
00335
00336 if (!thee->setUseAqua) thee->useAqua = 0;
00337
00338 return rc;
00339 }
00340
00341 VPUBLIC void MGparm_copy(MGparm *thee, MGparm *parm) {
00342     int i;
00343
00344     VASSERT(thee != VNULL);
00345     VASSERT(parm != VNULL);
00346
00347     thee->type = parm->type;
00348     thee->parsed = parm->parsed;
00349
00350     /* *** GENERIC PARAMETERS *** */
00351     for (i=0; i<3; i++) thee->dime[i] = parm->dime[i];
00352     thee->setdime = parm->setdime;
00353     thee->chgm = parm->chgm;
00354     thee->setchgm = parm->setchgm;
00355     thee->chgs = parm->chgs;
00356
00357     /* *** TYPE 0 PARMS *** */
00358     thee->nlev = parm->nlev;
00359     thee->setnlev = parm->setnlev;
00360     thee->etol = parm->etol;
00361     thee->setetol = parm->setetol;
00362     for (i=0; i<3; i++) thee->grid[i] = parm->grid[i];
00363     thee->setgrid = parm->setgrid;
00364     for (i=0; i<3; i++) thee->glen[i] = parm->glen[i];
00365     thee->setglen = parm->setglen;
00366     thee->cmeth = parm->cmeth;
00367     for (i=0; i<3; i++) thee->center[i] = parm->center[i];
00368     thee->setgcent = parm->setgcent;
00369 }

```

```

00371     thee->centmol = parm->centmol;
00372
00373     /* *** TYPE 1 & 2 PARMS *** */
00374     for (i=0; i<3; i++) thee->cglen[i] = parm->cglen[i];
00375     thee->setcglen = parm->setcglen;
00376     for (i=0; i<3; i++) thee->fglen[i] = parm->fglen[i];
00377     thee->setfglen = parm->setfglen;
00378     thee->ccmeth = parm->ccmeth;
00379     for (i=0; i<3; i++) thee->ccenter[i] = parm->ccenter[i];
00380     thee->setcgcent = parm->setcgcent;
00381     thee->ccentmol = parm->ccentmol;
00382     thee->fcmeth = parm->fcmeth;
00383     for (i=0; i<3; i++) thee->fcenter[i] = parm->fcenter[i];
00384     thee->setfgcent = parm->setfgcent;
00385     thee->fcentmol = parm->fcentmol;
00386
00387     /* *** TYPE 2 PARMS *** */
00388     for (i=0; i<3; i++)
00389         thee->partDisjCenter[i] = parm->partDisjCenter[i];
00390     for (i=0; i<3; i++)
00391         thee->partDisjLength[i] = parm->partDisjLength[i];
00392     for (i=0; i<6; i++)
00393         thee->partDisjOwnSide[i] = parm->partDisjOwnSide[i];
00394     for (i=0; i<3; i++) thee->pdime[i] = parm->pdime[i];
00395     thee->setpdime = parm->setpdime;
00396     thee->proc_rank = parm->proc_rank;
00397     thee->setrank = parm->setrank;
00398     thee->proc_size = parm->proc_size;
00399     thee->setsize = parm->setsize;
00400     thee->ofrac = parm->ofrac;
00401     thee->setofrac = parm->setofrac;
00402     thee->setasync = parm->setasync;
00403     thee->async = parm->async;
00404
00405     thee->nonlntype = parm->nonlntype;
00406     thee->setnonlntype = parm->setnonlntype;
00407
00408     thee->method = parm->method;
00409     thee->method = parm->method;
00410
00411     thee->useAqua = parm->useAqua;
00412     thee->setUseAqua = parm->setUseAqua;
00413 }
00414
00415 VPRIVATE Vrc_Codes MGparm_parseDIME(MGparm *thee, Vio *sock) {
00416
00417     char tok[VMAX_BUFSIZE];
00418     int ti;
00419
00420     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00421     if (sscanf(tok, "%d", &ti) == 0) {
00422         Vnm_print(2, "parseMG: Read non-integer (%s) while parsing DIME \
00423 keyword!\n", tok);
00424         return VRC_WARNING;
00425     } else thee->dime[0] = ti;
00426     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00427     if (sscanf(tok, "%d", &ti) == 0) {
00428         Vnm_print(2, "Nosh: Read non-integer (%s) while parsing DIME \
00429 keyword!\n", tok);
00430         return VRC_WARNING;
00431     } else thee->dime[1] = ti;
00432     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00433     if (sscanf(tok, "%d", &ti) == 0) {
00434         Vnm_print(2, "Nosh: Read non-integer (%s) while parsing DIME \
00435 keyword!\n", tok);
00436         return VRC_WARNING;
00437     } else thee->dime[2] = ti;
00438     thee->setdime = 1;
00439     return VRC_SUCCESS;
00440
00441     VERROR1:
00442     Vnm_print(2, "parseMG: ran out of tokens!\n");
00443     return VRC_WARNING;
00444 }
00445
00446 VPRIVATE Vrc_Codes MGparm_parseCHGM(MGparm *thee, Vio *sock) {
00447
00448     char tok[VMAX_BUFSIZE];
00449     Vchrg_Meth ti;
00450
00451     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);

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```

00452     if (sscanf(tok, "%d", (int*)&ti)) == 1) {
00453         thee->chgm = ti;
00454         thee->setchgm = 1;
00455         Vnm_print(2, "Nosh: Warning -- parsed deprecated statment \"chgm %d\".\n", ti);
00456         Vnm_print(2, "Nosh: Please use \"chgm \");
00457         switch (thee->chgm) {
00458             case VCM_TRIL:
00459                 Vnm_print(2, "spl0");
00460                 break;
00461             case VCM_BSPL2:
00462                 Vnm_print(2, "spl2");
00463                 break;
00464             case VCM_BSPL4:
00465                 Vnm_print(2, "spl4");
00466                 break;
00467             default:
00468                 Vnm_print(2, "UNKNOWN");
00469                 break;
00470         }
00471         Vnm_print(2, "\" instead!\n");
00472         return VRC_SUCCESS;
00473     } else if (Vstring_strcasecmp(tok, "spl0") == 0) {
00474         thee->chgm = VCM_TRIL;
00475         thee->setchgm = 1;
00476         return VRC_SUCCESS;
00477     } else if (Vstring_strcasecmp(tok, "spl2") == 0) {
00478         thee->chgm = VCM_BSPL2;
00479         thee->setchgm = 1;
00480         return VRC_SUCCESS;
00481     } else if (Vstring_strcasecmp(tok, "spl4") == 0) {
00482         thee->chgm = VCM_BSPL4;
00483         thee->setchgm = 1;
00484         return VRC_SUCCESS;
00485     } else {
00486         Vnm_print(2, "Nosh: Unrecognized parameter (%s) when parsing \"
00487 chgm!\n", tok);
00488         return VRC_WARNING;
00489     }
00490     return VRC_WARNING;
00491
00492     VERROR1:
00493         Vnm_print(2, "parseMG: ran out of tokens!\n");
00494         return VRC_WARNING;
00495 }
00496
00497 VPRIVATE Vrc_Codes MGparm_parseNLEV(MGparm *thee, Vio *sock) {
00498
00499     char tok[VMAX_BUFSIZE];
00500     int ti;
00501
00502     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00503     if (sscanf(tok, "%d", &ti)) == 0) {
00504         Vnm_print(2, "Nosh: Read non-integer (%s) while parsing NLEV \"
00505 keyword!\n", tok);
00506         return VRC_WARNING;
00507     } else thee->nlev = ti;
00508     thee->setnlev = 1;
00509     return VRC_SUCCESS;
00510
00511     VERROR1:
00512         Vnm_print(2, "parseMG: ran out of tokens!\n");
00513         return VRC_WARNING;
00514 }
00515
00516 VPRIVATE Vrc_Codes MGparm_parseETOL(MGparm *thee, Vio *sock) {
00517
00518     char tok[VMAX_BUFSIZE];
00519     double tf;
00520
00521     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00522     if (sscanf(tok, "%lf", &tf)) == 0) {
00523         Vnm_print(2, "Nosh: Read non-float (%s) while parsing etol \"
00524 keyword!\n", tok);
00525         return VRC_WARNING;
00526     } else if (tf <= 0.0) {
00527         Vnm_print(2, "parseMG: etol must be greater than 0!\n");
00528         return VRC_WARNING;
00529     } else thee->etol = tf;
00530     thee->setetol = 1;
00531     return VRC_SUCCESS;
00532

```

```

00533     ERROR1:
00534         Vnm_print(2, "parseMG:  ran out of tokens!\n");
00535         return VRC_WARNING;
00536 }
00537
00538
00539 VPRIVATE Vrc_Codes MGparm_parseGRID(MGparm *thee, Vio *sock) {
00540
00541     char tok[VMAX_BUFSIZE];
00542     double tf;
00543
00544     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00545     if (sscanf(tok, "%lf", &tf) == 0) {
00546         Vnm_print(2, "Nosh:  Read non-float (%s) while parsing GRID \
00547 keyword!\n", tok);
00548         return VRC_WARNING;
00549     } else thee->grid[0] = tf;
00550     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00551     if (sscanf(tok, "%lf", &tf) == 0) {
00552         Vnm_print(2, "Nosh:  Read non-float (%s) while parsing GRID \
00553 keyword!\n", tok);
00554         return VRC_WARNING;
00555     } else thee->grid[1] = tf;
00556     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00557     if (sscanf(tok, "%lf", &tf) == 0) {
00558         Vnm_print(2, "Nosh:  Read non-float (%s) while parsing GRID \
00559 keyword!\n", tok);
00560         return VRC_WARNING;
00561     } else thee->grid[2] = tf;
00562     thee->setgrid = 1;
00563     return VRC_SUCCESS;
00564
00565     ERROR1:
00566         Vnm_print(2, "parseMG:  ran out of tokens!\n");
00567         return VRC_WARNING;
00568 }
00569
00570 VPRIVATE Vrc_Codes MGparm_parseGLEN(MGparm *thee, Vio *sock) {
00571
00572     char tok[VMAX_BUFSIZE];
00573     double tf;
00574
00575     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00576     if (sscanf(tok, "%lf", &tf) == 0) {
00577         Vnm_print(2, "Nosh:  Read non-float (%s) while parsing GLEN \
00578 keyword!\n", tok);
00579         return VRC_WARNING;
00580     } else thee->glen[0] = tf;
00581     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00582     if (sscanf(tok, "%lf", &tf) == 0) {
00583         Vnm_print(2, "Nosh:  Read non-float (%s) while parsing GLEN \
00584 keyword!\n", tok);
00585         return VRC_WARNING;
00586     } else thee->glen[1] = tf;
00587     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00588     if (sscanf(tok, "%lf", &tf) == 0) {
00589         Vnm_print(2, "Nosh:  Read non-float (%s) while parsing GLEN \
00590 keyword!\n", tok);
00591         return VRC_WARNING;
00592     } else thee->glen[2] = tf;
00593     thee->setglen = 1;
00594     return VRC_SUCCESS;
00595
00596     ERROR1:
00597         Vnm_print(2, "parseMG:  ran out of tokens!\n");
00598         return VRC_WARNING;
00599 }
00600
00601 VPRIVATE Vrc_Codes MGparm_parseGAMMA(MGparm *thee, Vio *sock) {
00602
00603     char tok[VMAX_BUFSIZE];
00604
00605     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00606     Vnm_print(2, "parseMG:  GAMMA keyword deprecated!\n");
00607     Vnm_print(2, "parseMG:  If you are using PyMOL or VMD and still seeing this message,\n");
00608     Vnm_print(2, "parseMG:  please contact the developers of those programs regarding this message.\n");
00609     return VRC_SUCCESS;
00610
00611     ERROR1:
00612         Vnm_print(2, "parseMG:  ran out of tokens!\n");
00613         return VRC_WARNING;

```

```
00614 }
00615
00616 VPRIVATE Vrc_Codes MGparm_parseGCENT(MGparm *thee, Vio *sock) {
00617     char tok[VMAX_BUFSIZE];
00618     double tf;
00619     int ti;
00620
00621     /* If the next token isn't a float, it probably means we want to
00622      * center on a molecule */
00623     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00624     if (sscanf(tok, "%lf", &tf) == 0) {
00625         if (Vstring_strcasecmp(tok, "mol") == 0) {
00626             VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00627             if (sscanf(tok, "%d", &ti) == 0) {
00628                 Vnm_print(2, "Nosh: Read non-int (%s) while parsing \
00629 GCENT MOL keyword!\n", tok);
00630                 return VRC_WARNING;
00631             } else {
00632                 thee->cmeth = MCM_MOLECULE;
00633                 /* Subtract 1 here to convert user numbering (1, 2, 3, ...) into
00634                  array index */
00635                 thee->centmol = ti - 1;
00636             }
00637         } else {
00638             Vnm_print(2, "Nosh: Unexpected keyword (%s) while parsing \
00639 GCENT!\n", tok);
00640             return VRC_WARNING;
00641         }
00642     } else {
00643         thee->center[0] = tf;
00644         VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00645         if (sscanf(tok, "%lf", &tf) == 0) {
00646             Vnm_print(2, "Nosh: Read non-float (%s) while parsing \
00647 GCENT keyword!\n", tok);
00648             return VRC_WARNING;
00649         }
00650         thee->center[1] = tf;
00651         VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00652         if (sscanf(tok, "%lf", &tf) == 0) {
00653             Vnm_print(2, "Nosh: Read non-float (%s) while parsing \
00654 GCENT keyword!\n", tok);
00655             return VRC_WARNING;
00656         }
00657         thee->center[2] = tf;
00658     }
00659     thee->setgcent = 1;
00660     return VRC_SUCCESS;
00661 }
00662
00663 VERROR1:
00664     Vnm_print(2, "parseMG: ran out of tokens!\n");
00665     return VRC_WARNING;
00666 }
00667
00668 VPRIVATE Vrc_Codes MGparm_parseCGLEN(MGparm *thee, Vio *sock) {
00669     char tok[VMAX_BUFSIZE];
00670     double tf;
00671
00672     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00673     if (sscanf(tok, "%lf", &tf) == 0) {
00674         Vnm_print(2, "Nosh: Read non-float (%s) while parsing CGLEN \
00675 keyword!\n", tok);
00676         return VRC_WARNING;
00677     } else {
00678         thee->cglen[0] = tf;
00679         VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00680         if (sscanf(tok, "%lf", &tf) == 0) {
00681             Vnm_print(2, "Nosh: Read non-float (%s) while parsing CGLEN \
00682 keyword!\n", tok);
00683             return VRC_WARNING;
00684         } else {
00685             thee->cglen[1] = tf;
00686             VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00687             if (sscanf(tok, "%lf", &tf) == 0) {
00688                 Vnm_print(2, "Nosh: Read non-float (%s) while parsing CGLEN \
00689 keyword!\n", tok);
00690                 return VRC_WARNING;
00691             } else {
00692                 thee->cglen[2] = tf;
00693                 thee->setcglen = 1;
00694                 return VRC_SUCCESS;
00695             }
00696         }
00697     }
00698     VERROR1:
00699     Vnm_print(2, "parseMG: ran out of tokens!\n");
00700     return VRC_WARNING;
00701 }
```

```

00695     Vnm_print(2, "parseMG: ran out of tokens!\n");
00696     return VRC_WARNING;
00697 }
00698
00699 VPRIVATE Vrc_Codes MGparm_parseFGLEN(MGparm *thee, Vio *sock) {
00700     char tok[VMAX_BUFSIZE];
00701     double tf;
00702
00703     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00704     if (sscanf(tok, "%lf", &tf) == 0) {
00705         Vnm_print(2, "Nosh: Read non-float (%s) while parsing FGLEN \
00706 keyword!\n", tok);
00707         return VRC_WARNING;
00708     } else thee->fglen[0] = tf;
00709     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00710     if (sscanf(tok, "%lf", &tf) == 0) {
00711         Vnm_print(2, "Nosh: Read non-float (%s) while parsing FGLEN \
00712 keyword!\n", tok);
00713         return VRC_WARNING;
00714     } else thee->fglen[1] = tf;
00715     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00716     if (sscanf(tok, "%lf", &tf) == 0) {
00717         Vnm_print(2, "Nosh: Read non-float (%s) while parsing FGLEN \
00718 keyword!\n", tok);
00719         return VRC_WARNING;
00720     } else thee->fglen[2] = tf;
00721     thee->setfglen = 1;
00722     return VRC_SUCCESS;
00723 }
00724
00725 ERROR1:
00726     Vnm_print(2, "parseMG: ran out of tokens!\n");
00727     return VRC_WARNING;
00728 }
00729
00730 VPRIVATE Vrc_Codes MGparm_parseCGCENT(MGparm *thee, Vio *sock) {
00731     char tok[VMAX_BUFSIZE];
00732     double tf;
00733     int ti;
00734
00735     /* If the next token isn't a float, it probably means we want to
00736      * center on a molecule */
00737     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00738     if (sscanf(tok, "%lf", &tf) == 0) {
00739         if (Vstring_strcasecmp(tok, "mol") == 0) {
00740             VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00741             if (sscanf(tok, "%d", &ti) == 0) {
00742                 Vnm_print(2, "Nosh: Read non-int (%s) while parsing \
00743 CGCENT MOL keyword!\n", tok);
00744                 return VRC_WARNING;
00745             } else {
00746                 thee->ccmeth = MCM_MOLECULE;
00747                 /* Subtract 1 here to convert user numbering (1, 2, 3, ...) into
00748                  array index */
00749                 thee->ccentmol = ti - 1;
00750             }
00751         } else {
00752             Vnm_print(2, "Nosh: Unexpected keyword (%s) while parsing \
00753 CGCENT!\n", tok);
00754             return VRC_WARNING;
00755         }
00756     } else {
00757         thee->ccenter[0] = tf;
00758         VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00759         if (sscanf(tok, "%lf", &tf) == 0) {
00760             Vnm_print(2, "Nosh: Read non-float (%s) while parsing \
00761 CGCENT keyword!\n", tok);
00762             return VRC_WARNING;
00763         }
00764         thee->ccenter[1] = tf;
00765         VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00766         if (sscanf(tok, "%lf", &tf) == 0) {
00767             Vnm_print(2, "Nosh: Read non-float (%s) while parsing \
00768 CGCENT keyword!\n", tok);
00769             return VRC_WARNING;
00770         }
00771         thee->ccenter[2] = tf;
00772     }
00773     thee->setcgcent = 1;
00774     return VRC_SUCCESS;
00775 }

```

```

00776
00777     ERROR1:
00778         Vnm_print(2, "parseMG: ran out of tokens!\n");
00779         return VRC_WARNING;
00780 }
00781
00782 VPRIVATE Vrc_Codes MGparm_parseFGCENT(MGparm *thee, Vio *sock) {
00783
00784     char tok[VMAX_BUFSIZE];
00785     double tf;
00786     int ti;
00787
00788     /* If the next token isn't a float, it probably means we want to
00789      * center on a molecule */
00790     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00791     if (sscanf(tok, "%lf", &tf) == 0) {
00792         if (Vstring_strcasecmp(tok, "mol") == 0) {
00793             VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00794             if (sscanf(tok, "%d", &ti) == 0) {
00795                 Vnm_print(2, "Nosh: Read non-int (%s) while parsing \
00796 FGCENT MOL keyword!\n", tok);
00797                 return VRC_WARNING;
00798             } else {
00799                 thee->fcmeth = MCM_MOLECULE;
00800                 /* Subtract 1 here to convert user numbering (1, 2, 3, ...) into
00801                  array index */
00802                 thee->fcentmol = ti - 1;
00803             }
00804         } else {
00805             Vnm_print(2, "Nosh: Unexpected keyword (%s) while parsing \
00806 FGCENT!\n", tok);
00807             return VRC_WARNING;
00808         }
00809     } else {
00810         thee->fcenter[0] = tf;
00811         VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00812         if (sscanf(tok, "%lf", &tf) == 0) {
00813             Vnm_print(2, "Nosh: Read non-float (%s) while parsing \
00814 FGCENT keyword!\n", tok);
00815             return VRC_WARNING;
00816         }
00817         thee->fcenter[1] = tf;
00818         VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00819         if (sscanf(tok, "%lf", &tf) == 0) {
00820             Vnm_print(2, "Nosh: Read non-float (%s) while parsing \
00821 FGCENT keyword!\n", tok);
00822             return VRC_WARNING;
00823         }
00824         thee->fcenter[2] = tf;
00825     }
00826     thee->setfgcent = 1;
00827     return VRC_SUCCESS;
00828
00829     ERROR1:
00830         Vnm_print(2, "parseMG: ran out of tokens!\n");
00831         return VRC_WARNING;
00832 }
00833
00834 VPRIVATE Vrc_Codes MGparm_parsePDIME(MGparm *thee, Vio *sock) {
00835
00836     char tok[VMAX_BUFSIZE];
00837     int ti;
00838
00839     /* Read the number of grid points */
00840     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00841     if (sscanf(tok, "%d", &ti) == 0) {
00842         Vnm_print(2, "Nosh: Read non-integer (%s) while parsing PDIME \
00843 keyword!\n", tok);
00844         return VRC_WARNING;
00845     } else {
00846         thee->pdime[0] = ti;
00847     }
00848     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00849     if (sscanf(tok, "%d", &ti) == 0) {
00850         Vnm_print(2, "Nosh: Read non-integer (%s) while parsing PDIME \
00851 keyword!\n", tok);
00852         return VRC_WARNING;
00853     } else {
00854         thee->pdime[1] = ti;
00855     }
00856     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);

```



```

00857     if (sscanf(tok, "%d", &ti) == 0) {
00858         Vnm_print(2, "Nosh: Read non-integer (%s) while parsing PDIME \
00859 keyword!\n", tok);
00860         return VRC_WARNING;
00861     } else {
00862         thee->pdime[2] = ti;
00863     }
00864     thee->setpdime = 1;
00865     return VRC_SUCCESS;
00866
00867     VERROR1:
00868     Vnm_print(2, "parseMG: ran out of tokens!\n");
00869     return VRC_WARNING;
00870 }
00871
00872 VPRIVATE Vrc_Codes MGparm_parseOFRAC(MGparm *thee, Vio *sock) {
00873
00874     char tok[VMAX_BUFSIZE];
00875     double tf;
00876
00877     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00878     if (sscanf(tok, "%lf", &tf) == 0) {
00879         Vnm_print(2, "Nosh: Read non-int (%s) while parsing OFRAC \
00880 keyword!\n", tok);
00881         return VRC_WARNING;
00882     }
00883     thee->ofrac = tf;
00884     thee->setofrac = 1;
00885     return VRC_SUCCESS;
00886
00887     VERROR1:
00888     Vnm_print(2, "parseMG: ran out of tokens!\n");
00889     return VRC_WARNING;
00890 }
00891
00892 VPRIVATE Vrc_Codes MGparm_parseASYN(MGparm *thee, Vio *sock) {
00893
00894     char tok[VMAX_BUFSIZE];
00895     int ti;
00896
00897     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00898     if (sscanf(tok, "%i", &ti) == 0) {
00899         Vnm_print(2, "Nosh: Read non-integer (%s) while parsing ASYN \
00900 keyword!\n", tok);
00901         return VRC_WARNING;
00902     }
00903     thee->asyn = ti;
00904     thee->setasyn = 1;
00905     return VRC_SUCCESS;
00906
00907     VERROR1:
00908     Vnm_print(2, "parseMG: ran out of tokens!\n");
00909     return VRC_WARNING;
00910 }
00911
00912 VPRIVATE Vrc_Codes MGparm_parseUSEAQUA(MGparm *thee, Vio *sock) {
00913     Vnm_print(0, "Nosh: parsed useaqua\n");
00914     thee->useAqua = 1;
00915     thee->setUseAqua = 1;
00916     return VRC_SUCCESS;
00917 }
00918
00919 VPUBLIC Vrc_Codes MGparm_parseToken(MGparm *thee, char tok[VMAX_BUFSIZE],
00920     Vio *sock) {
00921
00922     if (thee == VNULL) {
00923         Vnm_print(2, "parseMG: got NULL thee!\n");
00924         return VRC_WARNING;
00925     }
00926     if (sock == VNULL) {
00927         Vnm_print(2, "parseMG: got NULL socket!\n");
00928         return VRC_WARNING;
00929     }
00930
00931     Vnm_print(0, "MGparm_parseToken: trying %s...\n", tok);
00932
00933     if (Vstring_strcasecmp(tok, "dime") == 0) {
00934         return MGparm_parseDIME(thee, sock);
00935     } else if (Vstring_strcasecmp(tok, "chgm") == 0) {
00936         return MGparm_parseCHGM(thee, sock);
00937     }

```

```

00938     } else if (Vstring_strcasecmp(tok, "nlev") == 0) {
00939         Vnm_print(2, "Warning: The 'nlev' keyword is now deprecated!\n");
00940         return MGparm_parseNLEV(thee, sock);
00941     } else if (Vstring_strcasecmp(tok, "etol") == 0) {
00942         return MGparm_parseETOL(thee, sock);
00943     } else if (Vstring_strcasecmp(tok, "grid") == 0) {
00944         return MGparm_parseGRID(thee, sock);
00945     } else if (Vstring_strcasecmp(tok, "glen") == 0) {
00946         return MGparm_parseGLEN(thee, sock);
00947     } else if (Vstring_strcasecmp(tok, "gcent") == 0) {
00948         return MGparm_parseGCENT(thee, sock);
00949     } else if (Vstring_strcasecmp(tok, "cglen") == 0) {
00950         return MGparm_parseCGLEN(thee, sock);
00951     } else if (Vstring_strcasecmp(tok, "fglen") == 0) {
00952         return MGparm_parseFGLEN(thee, sock);
00953     } else if (Vstring_strcasecmp(tok, "cgcent") == 0) {
00954         return MGparm_parseCGCENT(thee, sock);
00955     } else if (Vstring_strcasecmp(tok, "fgcent") == 0) {
00956         return MGparm_parseFGCENT(thee, sock);
00957     } else if (Vstring_strcasecmp(tok, "pdime") == 0) {
00958         return MGparm_parsePDIME(thee, sock);
00959     } else if (Vstring_strcasecmp(tok, "ofrac") == 0) {
00960         return MGparm_parseOFRAC(thee, sock);
00961     } else if (Vstring_strcasecmp(tok, "async") == 0) {
00962         return MGparm_parseASYNC(thee, sock);
00963     } else if (Vstring_strcasecmp(tok, "gamma") == 0) {
00964         return MGparm_parseGAMMA(thee, sock);
00965     } else if (Vstring_strcasecmp(tok, "useaqua") == 0) {
00966         return MGparm_parseUSEAQUA(thee, sock);
00967     } else {
00968         Vnm_print(2, "parseMG: Unrecognized keyword (%s)!\n", tok);
00969         return VRC_WARNING;
00970     }
00971
00972     return VRC_FAILURE;
00973
00974 }

```

9.32 src/generic/mgparm.h File Reference

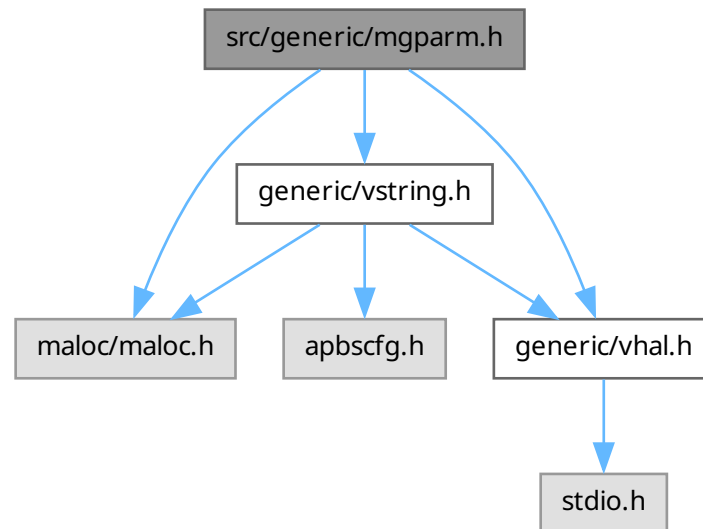
Contains declarations for class MGparm.

```

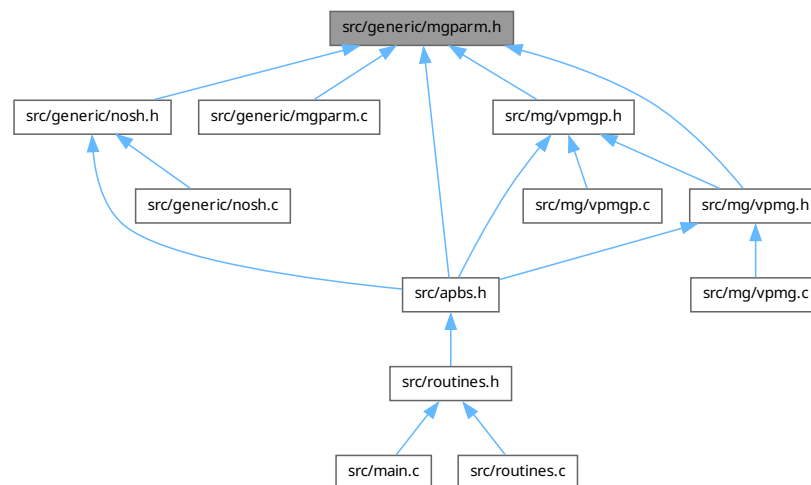
#include "malloc/malloc.h"
#include "generic/vhal.h"
#include "generic/vstring.h"

```

Include dependency graph for mgparm.h:



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [sMGparm](#)

Parameter structure for MG-specific variables from input files.

Typedefs

- typedef enum [eMGparm_CalcType](#) [MGparm_CalcType](#)
Declare MGparm_CalcType type.
- typedef enum [eMGparm_CentMeth](#) [MGparm_CentMeth](#)
Declare MGparm_CentMeth type.
- typedef struct [sMGparm](#) [MGparm](#)

Enumerations

- enum [eMGparm_CalcType](#) {
[MCT_MANUAL](#) =0 , [MCT_AUTO](#) =1 , [MCT_PARALLEL](#) =2 , [MCT_DUMMY](#) =3 ,
[MCT_NONE](#) =4 }
Calculation type.
- enum [eMGparm_CentMeth](#) { [MCM_POINT](#) =0 , [MCM_MOLECULE](#) =1 , [MCM_FOCUS](#) =2 }
Centering method.

Functions

- VEXTERNC int [MGparm_getNx](#) ([MGparm](#) *thee)
Get number of grid points in x direction.
- VEXTERNC int [MGparm_getNy](#) ([MGparm](#) *thee)
Get number of grid points in y direction.
- VEXTERNC int [MGparm_getNz](#) ([MGparm](#) *thee)
Get number of grid points in z direction.
- VEXTERNC double [MGparm_getHx](#) ([MGparm](#) *thee)
Get grid spacing in x direction (Å)
- VEXTERNC double [MGparm_getHy](#) ([MGparm](#) *thee)
Get grid spacing in y direction (Å)
- VEXTERNC double [MGparm_getHz](#) ([MGparm](#) *thee)
Get grid spacing in z direction (Å)
- VEXTERNC void [MGparm_setCenterX](#) ([MGparm](#) *thee, double x)
Set center x-coordinate.
- VEXTERNC void [MGparm_setCenterY](#) ([MGparm](#) *thee, double y)
Set center y-coordinate.
- VEXTERNC void [MGparm_setCenterZ](#) ([MGparm](#) *thee, double z)
Set center z-coordinate.
- VEXTERNC double [MGparm_getCenterX](#) ([MGparm](#) *thee)
Get center x-coordinate.
- VEXTERNC double [MGparm_getCenterY](#) ([MGparm](#) *thee)
Get center y-coordinate.
- VEXTERNC double [MGparm_getCenterZ](#) ([MGparm](#) *thee)
Get center z-coordinate.
- VEXTERNC [MGparm](#) * [MGparm_ctor](#) ([MGparm_CalcType](#) type)
Construct MGparm object.
- VEXTERNC [Vrc_Codes](#) [MGparm_ctor2](#) ([MGparm](#) *thee, [MGparm_CalcType](#) type)
FORTTRAN stub to construct MGparm object.
- VEXTERNC void [MGparm_dtor](#) ([MGparm](#) **thee)
Object destructor.

- VEXTERNC void `MGparm_dtor2` (`MGparm *thee`)
FORTTRAN stub for object destructor.
- VEXTERNC `Vrc_Codes` `MGparm_check` (`MGparm *thee`)
Consistency check for parameter values stored in object.
- VEXTERNC void `MGparm_copy` (`MGparm *thee`, `MGparm *parm`)
Copy MGparm object into thee.
- VEXTERNC `Vrc_Codes` `MGparm_parseToken` (`MGparm *thee`, `char tok[VMAX_BUFSIZE]`, `Vio *sock`)
Parse an MG keyword from an input file.

9.32.1 Detailed Description

Contains declarations for class `MGparm`.

Version

\$Id\$

Author

Nathan A. Baker

Attention

```
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*
*

```

Definition in file [mgparm.h](#).

9.32.2 Typedef Documentation

9.32.2.1 MGparm

typedef struct [sMGparm](#) [MGparm](#)

Definition at line 203 of file [mgparm.h](#).

9.33 mgparm.h

[Go to the documentation of this file.](#)

```

00001
00064 #ifndef _MGPARAM_H_
00065 #define _MGPARAM_H_
00066
00067 /* Generic header files */
00068 #include "malloc/malloc.h"
00069
00070 #include "generic/vhal.h"
00071 #include "generic/vstring.h"
00072
00077 enum eMGparm_CalcType {
00078     MCT_MANUAL=0,
00079     MCT_AUTO=1,
00080     MCT_PARALLEL=2,
00081     MCT_DUMMY=3,
00082     MCT_NONE=4
00083 };
00084
00089 typedef enum eMGparm_CalcType MGparm_CalcType;
00090
00095 enum eMGparm_CentMeth {
00096     MCM_POINT=0,
00097     MCM_MOLECULE=1,
00098     MCM_FOCUS=2
00099 };
00100
00105 typedef enum eMGparm_CentMeth MGparm_CentMeth;
00114 struct sMGparm {
00115
00116     MGparm_CalcType type;
00117     int parsed;
00119     /* *** GENERIC PARAMETERS *** */
00120     int dime[3];
00121     int setdime;
00122     Vchrg_Meth chgm;
00123     int setchgm;
00124     Vchrg_Src chgs;
00127     /* *** TYPE 0 PARAMETERS (SEQUENTIAL MANUAL) *** */
00128     int nlev;
00130     int setnlev;
00131     double etol;
00132     int setetol;
00133     double grid[3];
00134     int setgrid;
00135     double glen[3];
00136     int setglen;
00137     MGparm_CentMeth cmeth;
00138     double center[3];
00146     int centmol;
00149     int setgcent;
00151     /* ***** TYPE 1 & 2 PARAMETERS (SEQUENTIAL & PARALLEL AUTO-FOCUS) *** */
00152     double cglen[3];
00153     int setcglen;
00154     double fglen[3];

```

```

00155     int  setfglen;
00156     MGparm_CentMeth ccmeth;
00157     double ccenter[3];
00158     int  ccentmol;
00161     int  setcgcent;
00162     MGparm_CentMeth fcmeth;
00163     double fcenter[3];
00164     int  fcentmol;
00167     int  setfgcent;
00170     /* ***** TYPE 2 PARAMETERS (PARALLEL AUTO-FOCUS) ***** */
00171     double partDisjCenter[3];
00173     double partDisjLength[3];
00175     int  partDisjOwnSide[6];
00178     int  pdime[3];
00179     int  setpdime;
00180     int  proc_rank;
00181     int  setrank;
00182     int  proc_size;
00183     int  setsize;
00184     double ofrac;
00185     int  setofrac;
00186     int  async;
00187     int  setasync;
00189     int  nonlintype;
00190     int  setnonlintype;
00192     int  method;
00193     int  setmethod;
00195     int  useAqua;
00196     int  setUseAqua;
00197 };
00198
00203 typedef struct sMGparm MGparm;
00204
00211 VEXTERNC int  MGparm_getNx(MGparm *thee);
00212
00219 VEXTERNC int  MGparm_getNy(MGparm *thee);
00220
00227 VEXTERNC int  MGparm_getNz(MGparm *thee);
00228
00235 VEXTERNC double MGparm_getHx(MGparm *thee);
00236
00243 VEXTERNC double MGparm_getHy(MGparm *thee);
00244
00251 VEXTERNC double MGparm_getHz(MGparm *thee);
00252
00259 VEXTERNC void  MGparm_setCenterX(MGparm *thee, double x);
00260
00267 VEXTERNC void  MGparm_setCenterY(MGparm *thee, double y);
00268
00275 VEXTERNC void  MGparm_setCenterZ(MGparm *thee, double z);
00276
00283 VEXTERNC double MGparm_getCenterX(MGparm *thee);
00284
00291 VEXTERNC double MGparm_getCenterY(MGparm *thee);
00292
00299 VEXTERNC double MGparm_getCenterZ(MGparm *thee);
00300
00307 VEXTERNC MGparm*  MGparm_ctor(MGparm_CalcType type);
00308
00316 VEXTERNC Vrc_Codes  MGparm_ctor2(MGparm *thee, MGparm_CalcType type);
00317
00323 VEXTERNC void  MGparm_dtor(MGparm **thee);
00324
00330 VEXTERNC void  MGparm_dtor2(MGparm *thee);
00331
00338 VEXTERNC Vrc_Codes  MGparm_check(MGparm *thee);
00339
00346 VEXTERNC void  MGparm_copy(MGparm *thee, MGparm *parm);
00347
00357 VEXTERNC Vrc_Codes  MGparm_parseToken(MGparm *thee, char tok[VMAX_BUFSIZE],
00358     Vio *sock);
00359
00360 #endif
00361

```

9.34 src/generic/nosh.c File Reference

Class NOsh methods.

- Returns path to specified kappa map.*
- VPUBLIC char * [NOsh_getPotpath](#) (NOsh *thee, int imol)
- Returns path to specified potential map.*
- VPUBLIC char * [NOsh_getChargepath](#) (NOsh *thee, int imol)
- Returns path to specified charge distribution map.*
- VPUBLIC NOsh_calc * [NOsh_getCalc](#) (NOsh *thee, int icalc)
- Returns specified calculation object.*
- VPUBLIC int [NOsh_getDielfmt](#) (NOsh *thee, int i)
- Returns format of specified dielectric map.*
- VPUBLIC int [NOsh_getKappafmt](#) (NOsh *thee, int i)
- Returns format of specified kappa map.*
- VPUBLIC int [NOsh_getPotfmt](#) (NOsh *thee, int i)
- Returns format of specified potential map.*
- VPUBLIC int [NOsh_getChargefmt](#) (NOsh *thee, int i)
- Returns format of specified charge map.*
- VPUBLIC NOsh_PrintType [NOsh_printWhat](#) (NOsh *thee, int iprint)
- Return an integer ID of the observable to print (.).*
- VPUBLIC int [NOsh_printNarg](#) (NOsh *thee, int iprint)
- Return number of arguments to PRINT statement (.).*
- VPUBLIC int [NOsh_elec2calc](#) (NOsh *thee, int icalc)
- Return the name of an elec statement.*
- VPUBLIC int [NOsh_apol2calc](#) (NOsh *thee, int icalc)
- Return the name of an apol statement.*
- VPUBLIC char * [NOsh_elecname](#) (NOsh *thee, int ielec)
- Return an integer mapping of an ELEC statement to a calculation ID (.).*
- VPUBLIC int [NOsh_printOp](#) (NOsh *thee, int iprint, int iarg)
- Return integer ID for specified operation (.).*
- VPUBLIC int [NOsh_printCalc](#) (NOsh *thee, int iprint, int iarg)
- Return calculation ID for specified PRINT statement (.).*
- VPUBLIC NOsh * [NOsh_ctor](#) (int rank, int size)
- Construct NOsh.*
- VPUBLIC int [NOsh_ctor2](#) (NOsh *thee, int rank, int size)
- FORTTRAN stub to construct NOsh.*
- VPUBLIC void [NOsh_dtor](#) (NOsh **thee)
- Object destructor.*
- VPUBLIC void [NOsh_dtor2](#) (NOsh *thee)
- FORTTRAN stub for object destructor.*
- VPUBLIC NOsh_calc * [NOsh_calc_ctor](#) (NOsh_CalcType calctype)
- Construct NOsh_calc.*
- VPUBLIC void [NOsh_calc_dtor](#) (NOsh_calc **thee)
- Object destructor.*
- VPUBLIC int [NOsh_calc_copy](#) (NOsh_calc *thee, NOsh_calc *source)
- Copy NOsh_calc object into thee.*
- VPUBLIC int [NOsh_parseInputFile](#) (NOsh *thee, char *filename)
- Parse an input file only from a file.*
- VPUBLIC int [NOsh_parseInput](#) (NOsh *thee, Vio *sock)
- Parse an input file from a socket.*

- VPRIVATE int `NOsh_parseREAD_MOL` (`NOsh *thee`, `Vio *sock`)
- VPRIVATE int `NOsh_parseREAD_PARM` (`NOsh *thee`, `Vio *sock`)
- VPRIVATE int `NOsh_parseREAD_DIEL` (`NOsh *thee`, `Vio *sock`)
- VPRIVATE int `NOsh_parseREAD_KAPPA` (`NOsh *thee`, `Vio *sock`)
- VPRIVATE int `NOsh_parseREAD_POTENTIAL` (`NOsh *thee`, `Vio *sock`)
- VPRIVATE int `NOsh_parseREAD_CHARGE` (`NOsh *thee`, `Vio *sock`)
- VPRIVATE int `NOsh_parseREAD_MESH` (`NOsh *thee`, `Vio *sock`)
- VPUBLIC int `NOsh_setupElecCalc` (`NOsh *thee`, `Valist *alist[NOSH_MAXMOL]`)
Setup the series of electrostatics calculations.
- VPUBLIC int `NOsh_setupApolCalc` (`NOsh *thee`, `Valist *alist[NOSH_MAXMOL]`)
Setup the series of non-polar calculations.

9.34.1 Detailed Description

Class NOsh methods.

Author

Nathan Baker

Version

\$Id\$

Attention

```
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*

```

Definition in file [nosh.c](#).

9.34.2 Function Documentation

9.34.2.1 NOsh_parseAPOL()

```

VPUBLIC int NOsh_parseAPOL (
    NOsh * thee,
    Vio * sock,
    NOsh_calc * elec )

```

Definition at line [2508](#) of file [nosh.c](#).

9.34.2.2 NOsh_parseAPOLAR()

```

VPRIVATE int NOsh_parseAPOLAR (
    NOsh * thee,
    Vio * sock )

```

Definition at line [1313](#) of file [nosh.c](#).

9.34.2.3 NOsh_parseBEM()

```

VPUBLIC int NOsh_parseBEM (
    NOsh * thee,
    Vio * sock,
    NOsh_calc * elec )

```

Definition at line [2845](#) of file [nosh.c](#).

9.34.2.4 NOsh_parseELEC()

```

VPRIVATE int NOsh_parseELEC (
    NOsh * thee,
    Vio * sock )

```

Definition at line [1187](#) of file [nosh.c](#).

9.34.2.5 NOsh_parseFEM()

```

VPUBLIC int NOsh_parseFEM (
    NOsh * thee,
    Vio * sock,
    NOsh_calc * elec )

```

Definition at line [2385](#) of file [nosh.c](#).

9.34.2.6 NOsh_parseGEOFLOW()

```

VPUBLIC int NOsh_parseGEOFLOW (
    NOsh * thee,

```

```
Vio * sock,  
    NOsh_calc * elec )
```

Definition at line 2934 of file [nosh.c](#).

9.34.2.7 NOsh_parseMG()

```
VPUBLIC int NOsh_parseMG (  
    NOsh * thee,  
    Vio * sock,  
    NOsh_calc * elec )
```

Definition at line 1510 of file [nosh.c](#).

9.34.2.8 NOsh_parsePBAM()

```
VPUBLIC int NOsh_parsePBAM (  
    NOsh * thee,  
    Vio * sock,  
    NOsh_calc * elec )
```

Definition at line 3048 of file [nosh.c](#).

9.34.2.9 NOsh_parsePBSAM()

```
VPUBLIC int NOsh_parsePBSAM (  
    NOsh * thee,  
    Vio * sock,  
    NOsh_calc * elec )
```

Definition at line 3166 of file [nosh.c](#).

9.34.2.10 NOsh_parsePRINT()

```
VPRIVATE int NOsh_parsePRINT (  
    NOsh * thee,  
    Vio * sock )
```

Definition at line 1021 of file [nosh.c](#).

9.34.2.11 NOsh_parseREAD()

```
VPRIVATE int NOsh_parseREAD (  
    NOsh * thee,  
    Vio * sock )
```

Definition at line 970 of file [nosh.c](#).

9.34.2.12 NOsh_parseREAD_CHARGE()

```
VPRIVATE int NOsh_parseREAD_CHARGE (  
    NOsh * thee,  
    Vio * sock )
```

Definition at line 884 of file [nosh.c](#).

9.34.2.13 NOsh_parseREAD_DIEL()

```
VPRIVATE int NOsh_parseREAD_DIEL (  
    NOsh * thee,  
    Vio * sock )
```

Definition at line 739 of file [nosh.c](#).

9.34.2.14 NOsh_parseREAD_KAPPA()

```
VPRIVATE int NOsh_parseREAD_KAPPA (
    NOsh * thee,
    Vio * sock )
```

Definition at line 793 of file [nosh.c](#).

9.34.2.15 NOsh_parseREAD_MESH()

```
VPRIVATE int NOsh_parseREAD_MESH (
    NOsh * thee,
    Vio * sock )
```

Definition at line 930 of file [nosh.c](#).

9.34.2.16 NOsh_parseREAD_MOL()

```
VPRIVATE int NOsh_parseREAD_MOL (
    NOsh * thee,
    Vio * sock )
```

Definition at line 598 of file [nosh.c](#).

9.34.2.17 NOsh_parseREAD_PARM()

```
VPRIVATE int NOsh_parseREAD_PARM (
    NOsh * thee,
    Vio * sock )
```

Definition at line 675 of file [nosh.c](#).

9.34.2.18 NOsh_parseREAD_POTENTIAL()

```
VPRIVATE int NOsh_parseREAD_POTENTIAL (
    NOsh * thee,
    Vio * sock )
```

Definition at line 839 of file [nosh.c](#).

9.34.2.19 NOsh_setupCalcAPOL()

```
VPRIVATE int NOsh_setupCalcAPOL (
    NOsh * thee,
    NOsh_calc * elec )
```

Definition at line 2581 of file [nosh.c](#).

9.34.2.20 NOsh_setupCalcBEM()

```
VPRIVATE int NOsh_setupCalcBEM (
    NOsh * thee,
    NOsh_calc * elec )
```

Definition at line 1638 of file [nosh.c](#).

9.34.2.21 NOsh_setupCalcBEMMANUAL()

```
VPRIVATE int NOsh_setupCalcBEMMANUAL (
    NOsh * thee,
    NOsh_calc * elec )
```

Definition at line 2612 of file [nosh.c](#).

9.34.2.22 NOsh_setupCalcFEM()

```
VPRIVATE int NOsh_setupCalcFEM (
    NOsh * thee,
    NOsh_calc * elec )
```

Definition at line 1722 of file [nosh.c](#).

9.34.2.23 NOsh_setupCalcFEMANUAL()

```
VPRIVATE int NOsh_setupCalcFEMANUAL (
    NOsh * thee,
    NOsh_calc * elec )
```

Definition at line 2471 of file [nosh.c](#).

9.34.2.24 NOsh_setupCalcGEOFLOW()

```
VPRIVATE int NOsh_setupCalcGEOFLOW (
    NOsh * thee,
    NOsh_calc * elec )
```

Definition at line 1666 of file [nosh.c](#).

9.34.2.25 NOsh_setupCalcGEOFLOWMANUAL()

```
VPRIVATE int NOsh_setupCalcGEOFLOWMANUAL (
    NOsh * thee,
    NOsh_calc * elec )
```

Definition at line 2677 of file [nosh.c](#).

9.34.2.26 NOsh_setupCalcMG()

```
VPRIVATE int NOsh_setupCalcMG (
    NOsh * thee,
    NOsh_calc * elec )
```

Definition at line 1603 of file [nosh.c](#).

9.34.2.27 NOsh_setupCalcMGAUTO()

```
VPUBLIC int NOsh_setupCalcMGAUTO (
    NOsh * thee,
    NOsh_calc * elec )
```

Definition at line 1815 of file [nosh.c](#).

9.34.2.28 NOsh_setupCalcMGMANUAL()

```
VPRIVATE int NOsh_setupCalcMGMANUAL (
    NOsh * thee,
    NOsh_calc * elec )
```

Definition at line 1747 of file [nosh.c](#).

9.34.2.29 NOsh_setupCalcMGPARA()

```
VPUBLIC int NOsh_setupCalcMGPARA (
    NOsh * thee,
    NOsh_calc * elec )
```

Definition at line 2090 of file [nosh.c](#).

9.34.2.30 NOsh_setupCalcPBAM()

```
VPRIVATE int NOsh_setupCalcPBAM (
    NOsh * thee,
    NOsh_calc * elec )
```

Definition at line 1686 of file [nosh.c](#).

9.34.2.31 NOsh_setupCalcPBAMAUTO()

```
VPRIVATE int NOsh_setupCalcPBAMAUTO (
    NOsh * thee,
    NOsh_calc * elec )
```

Definition at line 2735 of file [nosh.c](#).

9.34.2.32 NOsh_setupCalcPBSAM()

```
VPRIVATE int NOsh_setupCalcPBSAM (
    NOsh * thee,
    NOsh_calc * elec )
```

Definition at line 1704 of file [nosh.c](#).

9.34.2.33 NOsh_setupCalcPBSAMAUTO()

```
VPRIVATE int NOsh_setupCalcPBSAMAUTO (
    NOsh * thee,
    NOsh_calc * elec )
```

Definition at line 2786 of file [nosh.c](#).

9.35 nosh.c

[Go to the documentation of this file.](#)

```
00001
00057 #include "nosh.h"
00058
00059 VEMBED(rcsid="$Id$")
00060
00061
00062 VPRIVATE int NOsh_parseREAD(
00063     NOsh *thee,
00064     Vio *sock);
00065
00066 VPRIVATE int NOsh_parsePRINT(
00067     NOsh *thee,
00068     Vio *sock);
00069
00070 VPRIVATE int NOsh_parseELEC(
00071     NOsh *thee,
00072     Vio *sock
00073 );
00074
00075 VPRIVATE int NOsh_parseAPOLAR(
00076     NOsh *thee,
00077     Vio *sock
00078 );
00079
00080 VEXTERNC int NOsh_parseFEM(
00081     NOsh *thee,
00082     Vio *sock,
00083     NOsh_calc *elec
00084 );
00085
00086 VEXTERNC int NOsh_parseMG(
00087     NOsh *thee,
00088     Vio *sock,
00089     NOsh_calc *elec
00090 );
```

```
00091
00092 VEXTERNC int NOsh_parseBEM(
00093     NOsh *thee,
00094     Vio *sock,
00095     NOsh_calc *elec
00096 );
00097
00098 VEXTERNC int NOsh_parseGEOFLOW(
00099     NOsh *thee,
00100     Vio *sock,
00101     NOsh_calc *elec
00102 );
00103
00104 VEXTERNC int NOsh_parsePBAM(
00105     NOsh *thee,
00106     Vio *sock,
00107     NOsh_calc *elec
00108 );
00109
00110 VEXTERNC int NOsh_parsePBSAM(
00111     NOsh *thee,
00112     Vio *sock,
00113     NOsh_calc *elec
00114 );
00115
00116 VEXTERNC int NOsh_parseAPOL(
00117     NOsh *thee,
00118     Vio *sock,
00119     NOsh_calc *elec
00120 );
00121
00122 VPRIVATE int NOsh_setupCalcMG(
00123     NOsh *thee,
00124     NOsh_calc *elec
00125 );
00126
00127
00128 VPRIVATE int NOsh_setupCalcMGAUTO(
00129     NOsh *thee,
00130     NOsh_calc *elec
00131 );
00132
00133 VPRIVATE int NOsh_setupCalcMGMANUAL(
00134     NOsh *thee,
00135     NOsh_calc *elec
00136 );
00137
00138 VPRIVATE int NOsh_setupCalcMGPARA(
00139     NOsh *thee,
00140     NOsh_calc *elec
00141 );
00142
00143 VPRIVATE int NOsh_setupCalcFEM(
00144     NOsh *thee,
00145     NOsh_calc *elec
00146 );
00147
00148 VPRIVATE int NOsh_setupCalcFEMANUAL(
00149     NOsh *thee,
00150     NOsh_calc *elec
00151 );
00152
00153 VPRIVATE int NOsh_setupCalcBEM(
00154     NOsh *thee,
00155     NOsh_calc *elec
00156 );
00157
00158 VPRIVATE int NOsh_setupCalcGEOFLOW(
00159     NOsh *thee,
00160     NOsh_calc *elec
00161 );
00162
00163 VPRIVATE int NOsh_setupCalcPBAM(
00164     NOsh *thee,
00165     NOsh_calc *elec
00166 );
00167
00168 VPRIVATE int NOsh_setupCalcPBSAM(
00169     NOsh *thee,
00170     NOsh_calc *elec
00171 );
```



```

00172
00173 VPRIVATE int NOsh_setupCalcBEMMANUAL(
00174     NOsh *thee,
00175     NOsh_calc *elec
00176 );
00177
00178 VPRIVATE int NOsh_setupCalcGEOFLOWMANUAL(
00179     NOsh *thee,
00180     NOsh_calc *elec
00181 );
00182
00183 VPRIVATE int NOsh_setupCalcPBAMAUTO(
00184     NOsh *thee,
00185     NOsh_calc *elec
00186 );
00187
00188 VPRIVATE int NOsh_setupCalcPBSAMAUTO(
00189     NOsh *thee,
00190     NOsh_calc *elec
00191 );
00192
00193 VPRIVATE int NOsh_setupCalcAPOL(
00194     NOsh *thee,
00195     NOsh_calc *elec
00196 );
00197
00198 #if !defined(VINLINE_NOSH)
00199
00200 VPUBLIC char* NOsh_getMolpath(NOsh *thee, int imol) {
00201     VASSERT(thee != VNULL);
00202     VASSERT(imol < thee->nmol);
00203     return thee->molpath[imol];
00204 }
00205 VPUBLIC char* NOsh_getDielXpath(NOsh *thee, int imol) {
00206     VASSERT(thee != VNULL);
00207     VASSERT(imol < thee->nmol);
00208     return thee->dielXpath[imol];
00209 }
00210 VPUBLIC char* NOsh_getDielYpath(NOsh *thee, int imol) {
00211     VASSERT(thee != VNULL);
00212     VASSERT(imol < thee->nmol);
00213     return thee->dielYpath[imol];
00214 }
00215 VPUBLIC char* NOsh_getDielZpath(NOsh *thee, int imol) {
00216     VASSERT(thee != VNULL);
00217     VASSERT(imol < thee->nmol);
00218     return thee->dielZpath[imol];
00219 }
00220 VPUBLIC char* NOsh_getKappapath(NOsh *thee, int imol) {
00221     VASSERT(thee != VNULL);
00222     VASSERT(imol < thee->nmol);
00223     return thee->kappapath[imol];
00224 }
00225 VPUBLIC char* NOsh_getPotpath(NOsh *thee, int imol) {
00226     VASSERT(thee != VNULL);
00227     VASSERT(imol < thee->nmol);
00228     return thee->potpath[imol];
00229 }
00230 VPUBLIC char* NOsh_getChargepath(NOsh *thee, int imol) {
00231     VASSERT(thee != VNULL);
00232     VASSERT(imol < thee->nmol);
00233     return thee->chargepath[imol];
00234 }
00235 VPUBLIC NOsh_calc* NOsh_getCalc(NOsh *thee, int icalc) {
00236     VASSERT(thee != VNULL);
00237     VASSERT(icalc < thee->ncalc);
00238     return thee->calc[icalc];
00239 }
00240 VPUBLIC int NOsh_getDielfmt(NOsh *thee, int i) {
00241     VASSERT(thee != VNULL);
00242     VASSERT(i < thee->ndiel);
00243     return (thee->dielfmt[i]);
00244 }
00245 VPUBLIC int NOsh_getKappafmt(NOsh *thee, int i) {
00246     VASSERT(thee != VNULL);
00247     VASSERT(i < thee->nkappa);
00248     return (thee->kappafmt[i]);
00249 }
00250 VPUBLIC int NOsh_getPotfmt(NOsh *thee, int i) {
00251     VASSERT(thee != VNULL);
00252     VASSERT(i < thee->npot);

```

```

00253     return (thee->potfmt[i]);
00254 }
00255 VPUBLIC int NOsh_getChargefmt(NOsh *thee, int i) {
00256     VASSERT(thee != VNULL);
00257     VASSERT(i < thee->ncharge);
00258     return (thee->chargefmt[i]);
00259 }
00260
00261
00262 #endif /* if !defined(VINLINE_NOSH) */
00263
00264 VPUBLIC NOsh_printType NOsh_printWhat(NOsh *thee, int iprint) {
00265     VASSERT(thee != VNULL);
00266     VASSERT(iprint < thee->nprint);
00267     return thee->printwhat[iprint];
00268 }
00269
00270 VPUBLIC int NOsh_printNarg(NOsh *thee, int iprint) {
00271     VASSERT(thee != VNULL);
00272     VASSERT(iprint < thee->nprint);
00273     return thee->printnarg[iprint];
00274 }
00275
00276 VPUBLIC int NOsh_elec2calc(NOsh *thee, int icalc) {
00277     VASSERT(thee != VNULL);
00278     VASSERT(icalc < thee->ncalc);
00279     return thee->elec2calc[icalc];
00280 }
00281
00282 VPUBLIC int NOsh_apol2calc(NOsh *thee, int icalc) {
00283     VASSERT(thee != VNULL);
00284     VASSERT(icalc < thee->ncalc);
00285     return thee->apol2calc[icalc];
00286 }
00287
00288 VPUBLIC char* NOsh_elecname(NOsh *thee, int ielec) {
00289     VASSERT(thee != VNULL);
00290     VASSERT(ielec < thee->nelec + 1);
00291     return thee->elecname[ielec];
00292 }
00293
00294 VPUBLIC int NOsh_printOp(NOsh *thee, int iprint, int iarg) {
00295     VASSERT(thee != VNULL);
00296     VASSERT(iprint < thee->nprint);
00297     VASSERT(iarg < thee->printnarg[iprint]);
00298     return thee->printop[iprint][iarg];
00299 }
00300
00301 VPUBLIC int NOsh_printCalc(NOsh *thee, int iprint, int iarg) {
00302     VASSERT(thee != VNULL);
00303     VASSERT(iprint < thee->nprint);
00304     VASSERT(iarg < thee->printnarg[iprint]);
00305     return thee->printcalc[iprint][iarg];
00306 }
00307
00308 VPUBLIC NOsh* NOsh_ctor(int rank, int size) {
00309     /* Set up the structure */
00310     NOsh *thee = VNULL;
00311     thee = (NOsh*)Vmem_malloc(VNULL, 1, sizeof(NOsh) );
00312     VASSERT( thee != VNULL);
00313     VASSERT( NOsh_ctor2(thee, rank, size) );
00314     return thee;
00315 }
00316
00317 }
00318
00319 VPUBLIC int NOsh_ctor2(NOsh *thee, int rank, int size) {
00320     int i;
00321
00322     if (thee == VNULL) return 0;
00323
00324     thee->proc_rank = rank;
00325     thee->proc_size = size;
00326
00327     thee->ispara = 0;
00328     thee->parsed = 0;
00329
00330     thee->nmol = 0;
00331     thee->gotparm = 0;
00332     thee->ncharge = 0;

```

```

00334     thee->ndiel = 0;
00335     thee->nkappa = 0;
00336     thee->npot = 0;
00337     thee->nprint = 0;
00338
00339     for (i=0; i<NOSH_MAXCALC; i++) {
00340         thee->calc[i] = VNULL;
00341         thee->elec[i] = VNULL;
00342         thee->apol[i] = VNULL;
00343     }
00344     for (i=0; i<NOSH_MAXMOL; i++) {
00345         thee->alist[i] = VNULL;
00346     }
00347     thee->ncalc = 0;
00348     thee->nelec = 0;
00349     thee->napol = 0;
00350
00351     return 1;
00352 }
00353
00354 VPUBLIC void NOsh_dtor(NOsh **thee) {
00355     if ((*thee) != VNULL) {
00356         NOsh_dtor2(*thee);
00357         Vmem_free(VNULL, 1, sizeof(NOsh), (void **)thee);
00358         (*thee) = VNULL;
00359     }
00360 }
00361
00362 VPUBLIC void NOsh_dtor2(NOsh *thee) {
00363
00364     int i;
00365
00366     if (thee != VNULL) {
00367         for (i=0; i<(thee->ncalc); i++) NOsh_calc_dtor(&(thee->calc[i]));
00368         for (i=0; i<(thee->nelec); i++) NOsh_calc_dtor(&(thee->elec[i]));
00369         for (i=0; i<(thee->napol); i++) NOsh_calc_dtor(&(thee->apol[i]));
00370     }
00371 }
00372 }
00373
00374 VPUBLIC NOsh_calc* NOsh_calc_ctor(
00375     NOsh_CalcType calctype
00376 ) {
00377     NOsh_calc *thee;
00378     thee = (NOsh_calc *)Vmem_malloc(VNULL, 1, sizeof(NOsh_calc));
00379     thee->calctype = calctype;
00380
00381     thee->mgparm = VNULL;
00382     thee->femparm = VNULL;
00383     thee->apolparm = VNULL;
00384     thee->bemparm = VNULL;
00385     thee->geoflowparm = VNULL;
00386     thee->pbamparm = VNULL;
00387     thee->pbsamparm = VNULL;
00388
00389     switch (calctype) {
00390     case NCT_MG:
00391         thee->mgparm = MGparm_ctor(MCT_NONE);
00392         break;
00393     case NCT_FEM:
00394         thee->femparm = FEMparm_ctor(FCT_NONE);
00395         break;
00396     case NCT_APOL:
00397         thee->apolparm = APOLparm_ctor();
00398         break;
00399     case NCT_BEM:
00400         thee->bemparm = BEMparm_ctor(BCT_MANUAL);
00401         break;
00402     case NCT_GEOFLOW:
00403         thee->geoflowparm = GEOFLOWparm_ctor(GFCT_AUTO);
00404         thee->apolparm = APOLparm_ctor();
00405         break;
00406     case NCT_PBAM:
00407         thee->pbamparm = PBAMparm_ctor(PBAMCT_AUTO);
00408         break;
00409     case NCT_PBSAM:
00410         thee->pbamparm = PBAMparm_ctor(PBAMCT_AUTO);
00411         thee->pbsamparm = PBSAMparm_ctor(PBSAMCT_AUTO);
00412         break;
00413     default:
00414         Vnm_print(2, "NOsh_calc_ctor: unknown calculation type (%d)!\n",

```

```

00415             calctype);
00416             VASSERT(0);
00417         }
00418         thee->pbeparm = PBEparm_ctor();
00419     }
00420     return thee;
00421 }
00422
00423 VPUBLIC void NOsh_calc_dtor(
00424     NOsh_calc **thee
00425 ) {
00426
00427     NOsh_calc *calc = VNULL;
00428     calc = *thee;
00429     if (calc == VNULL) return;
00430
00431     switch (calc->calctype) {
00432     case NCT_MG:
00433         MGparm_dtor(&(calc->mgparm));
00434         break;
00435     case NCT_FEM:
00436         FEMparm_dtor(&(calc->femparm));
00437         break;
00438     case NCT_APOL:
00439         APOLparm_dtor(&(calc->apolparm));
00440         break;
00441     case NCT_BEM:
00442         BEMparm_dtor(&(calc->bemparm));
00443         break;
00444     case NCT_GEOFLOW:
00445         GEOFLOWparm_dtor(&(calc->geoflowparm));
00446         APOLparm_dtor(&(calc->apolparm));
00447         break;
00448     case NCT_PBAM:
00449         PBAMparm_dtor(&(calc->pbamparm));
00450         break;
00451     case NCT_PBSAM:
00452         PBAMparm_dtor(&(calc->pbamparm));
00453         PBSAMparm_dtor(&(calc->pbsamparm));
00454         break;
00455     default:
00456         Vnm_print(2, "NOsh_calc_ctor: unknown calculation type (%d)!\n",
00457             calc->calctype);
00458         VASSERT(0);
00459     }
00460     PBEparm_dtor(&(calc->pbeparm));
00461
00462     Vmem_free(VNULL, 1, sizeof(NOsh_calc), (void **)thee);
00463     calc = VNULL;
00464 }
00465
00466
00467 VPUBLIC int NOsh_calc_copy(
00468     NOsh_calc *thee,
00469     NOsh_calc *source
00470 ) {
00471
00472     VASSERT(thee != VNULL);
00473     VASSERT(source != VNULL);
00474     VASSERT(thee->calctype == source->calctype);
00475     if (source->mgparm != VNULL)
00476         MGparm_copy(thee->mgparm, source->mgparm);
00477     if (source->femparm != VNULL)
00478         FEMparm_copy(thee->femparm, source->femparm);
00479     if (source->bemparm != VNULL)
00480         BEMparm_copy(thee->bemparm, source->bemparm);
00481     if (source->pbeparm != VNULL)
00482         PBEparm_copy(thee->pbeparm, source->pbeparm);
00483     if (source->apolparm != VNULL)
00484         APOLparm_copy(thee->apolparm, source->apolparm);
00485     /*I think here is where the the geoflow changes get lost*/
00486     if (source->geoflowparm != VNULL)
00487         GEOFLOWparm_copy(thee->geoflowparm, source->geoflowparm);
00488     if (source->pbamparm != VNULL)
00489         PBAMparm_copy(thee->pbamparm, source->pbamparm);
00490     if (source->pbsamparm != VNULL)
00491         PBSAMparm_copy(thee->pbsamparm, source->pbsamparm);
00492
00493     return 1;
00494 }
00495

```

```

00496 }
00497
00498 VPUBLIC int NOsh_parseInputFile(
00499     NOsh *thee,
00500     char *filename
00501 ) {
00502
00503     Vio *sock;
00504     int rc;
00505
00506     sock = Vio_ctor("FILE", "ASC", VNULL, filename, "r");
00507     rc = NOsh_parseInput(thee, sock);
00508     Vio_dtor(&sock);
00509
00510     return rc;
00511 }
00512
00513 VPUBLIC int NOsh_parseInput(
00514     NOsh *thee,
00515     Vio *sock
00516 ) {
00517
00518     char *MCwhiteChars = " =,;\t\r\n";
00519     char *MCcommChars = "#%";
00520     char tok[VMAX_BUFSIZE];
00521
00522     if (thee == VNULL) {
00523         Vnm_print(2, "NOsh_parseInput: Got NULL thee!\n");
00524         return 0;
00525     }
00526
00527     if (sock == VNULL) {
00528         Vnm_print(2, "NOsh_parseInput: Got pointer to NULL socket!\n");
00529         Vnm_print(2, "NOsh_parseInput: The specified input file was not found!\n");
00530         return 0;
00531     }
00532
00533     if (thee->parsed) {
00534         Vnm_print(2, "NOsh_parseInput: Already parsed an input file!\n");
00535         return 0;
00536     }
00537
00538     if (Vio_accept(sock, 0) < 0) {
00539         Vnm_print(2, "NOsh_parseInput: Problem reading from socket!\n");
00540         return 0;
00541     }
00542
00543     /* Set up the whitespace and comment character definitions */
00544     Vio_setWhiteChars(sock, MCwhiteChars);
00545     Vio_setCommChars(sock, MCommChars);
00546
00547     /* We parse the file until we run out of tokens */
00548     Vnm_print(0, "NOsh_parseInput: Starting file parsing...\n");
00549     while (Vio_scanf(sock, "%s", tok) == 1) {
00550         /* At the highest level, we look for keywords that indicate functions like:
00551
00552         read => Read in a molecule file
00553         elec => Do an electrostatics calculation
00554         print => Print some results
00555         apolar => do a non-polar calculation
00556         quit => Quit
00557
00558         These cause the code to go to a lower-level parser routine which
00559         handles keywords specific to the particular function. Each
00560         lower-level parser routine then returns when it hits the "end"
00561         keyword. Due to this simple layout, no nesting of these "function"
00562         sections is allowed.
00563         */
00564         if (Vstring_strcasecmp(tok, "read") == 0) {
00565             // printf("read\n");
00566             Vnm_print(0, "NOsh: Parsing READ section\n");
00567             if (!NOsh_parseREAD(thee, sock)) return 0;
00568             Vnm_print(0, "NOsh: Done parsing READ section \n");
00569             (nmol=%d, ndiel=%d, nkappa=%d, ncharge=%d, npot=%d)\n", thee->nmol, thee->ndiel,
00570             thee->nkappa, thee->ncharge, thee->npot);
00571         } else if (Vstring_strcasecmp(tok, "print") == 0) {
00572             Vnm_print(0, "NOsh: Parsing PRINT section\n");
00573             if (!NOsh_parsePRINT(thee, sock)) return 0;
00574             Vnm_print(0, "NOsh: Done parsing PRINT section\n");
00575         } else if (Vstring_strcasecmp(tok, "elec") == 0) {
00576             Vnm_print(0, "NOsh: Parsing ELEC section\n");

```

```
00577         if (!Nosh_parseELEC(thee, sock)) return 0;
00578         Vnm_print(0, "Nosh: Done parsing ELEC section (nelec = %d)\n",
00579                 thee->nelec);
00580     } else if (Vstring_strcasecmp(tok, "apolar") == 0) {
00581         Vnm_print(0, "Nosh: Parsing APOLAR section\n");
00582         if (!Nosh_parseAPOLAR(thee, sock)) return 0;
00583         Vnm_print(0, "Nosh: Done parsing APOLAR section (nelec = %d)\n",
00584                 thee->nelec);
00585     } else if (Vstring_strcasecmp(tok, "quit") == 0) {
00586         Vnm_print(0, "Nosh: Done parsing file (got QUIT)\n");
00587         break;
00588     } else {
00589         Vnm_print(2, "Nosh_parseInput: Ignoring undefined keyword %s!\n", tok);
00590     }
00591 }
00592
00593 thee->parsed = 1;
00594 return 1;
00595 }
00596
00597
00598 VPRIVATE int Nosh_parseREAD_MOL(Nosh *thee, Vio *sock) {
00599     char tok[VMAX_BUFSIZE], str[VMAX_BUFSIZE]="", strnew[VMAX_BUFSIZE]="";
00600     Nosh_MolFormat molfmt;
00601
00602     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00603     if (Vstring_strcasecmp(tok, "pqr") == 0) {
00604         molfmt = NMF_PQR;
00605         VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00606         if (tok[0]=='"') {
00607             strcpy(strnew, "");
00608             while (tok[strlen(tok)-1] != '"') {
00609                 strcat(str, tok);
00610                 strcat(str, " ");
00611                 VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00612             }
00613             strcat(str, tok);
00614             strncpy(strnew, str+1, strlen(str)-2);
00615             strcpy(tok, strnew);
00616         }
00617         Vnm_print(0, "Nosh: Storing molecule %d path %s\n",
00618                 thee->nmol, tok);
00619         thee->molfmt[thee->nmol] = molfmt;
00620         strncpy(thee->molpath[thee->nmol], tok, VMAX_ARGLEN);
00621         (thee->nmol)++;
00622     } else if (Vstring_strcasecmp(tok, "pdb") == 0) {
00623         molfmt = NMF_PDB;
00624         VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00625         if (tok[0]=='"') {
00626             strcpy(strnew, "");
00627             while (tok[strlen(tok)-1] != '"') {
00628                 strcat(str, tok);
00629                 strcat(str, " ");
00630                 VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00631             }
00632             strcat(str, tok);
00633             strncpy(strnew, str+1, strlen(str)-2);
00634             strcpy(tok, strnew);
00635         }
00636         Vnm_print(0, "Nosh: Storing molecule %d path %s\n",
00637                 thee->nmol, tok);
00638         thee->molfmt[thee->nmol] = molfmt;
00639         strncpy(thee->molpath[thee->nmol], tok, VMAX_ARGLEN);
00640         (thee->nmol)++;
00641     } else if (Vstring_strcasecmp(tok, "xml") == 0) {
00642         molfmt = NMF_XML;
00643         VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00644         if (tok[0]=='"') {
00645             strcpy(strnew, "");
00646             while (tok[strlen(tok)-1] != '"') {
00647                 strcat(str, tok);
00648                 strcat(str, " ");
00649                 VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00650             }
00651             strcat(str, tok);
00652             strncpy(strnew, str+1, strlen(str)-2);
00653             strcpy(tok, strnew);
00654         }
00655         Vnm_print(0, "Nosh: Storing molecule %d path %s\n",
00656                 thee->nmol, tok);
00657     }
```

```

00658     thee->molfmt[thee->nmol] = molfmt;
00659     strncpy(thee->molpath[thee->nmol], tok, VMAX_ARGLEN);
00660     (thee->nmol)++;
00661 } else {
00662     Vnm_print(2, "Nosh_parseREAD: Ignoring undefined mol format \
00663 %s!\n", tok);
00664 }
00665
00666     return 1;
00667
00668
00669 ERROR1:
00670     Vnm_print(2, "Nosh_parseREAD_MOL: Ran out of tokens while parsing READ section!\n");
00671     return 0;
00672
00673 }
00674
00675 VPRIVATE int Nosh_parseREAD_PARM(NOsh *thee, Vio *sock) {
00676
00677     char tok[VMAX_BUFSIZE], str[VMAX_BUFSIZE]="", strnew[VMAX_BUFSIZE]="";
00678     NOsh_ParmFormat parmfmt;
00679
00680     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00681     if (Vstring_strcasecmp(tok, "flat") == 0) {
00682         parmfmt = NPF_FLAT;
00683         VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00684         if (tok[0]=='"') {
00685             strcpy(strnew, "");
00686             while (tok[strlen(tok)-1] != '"') {
00687                 strcat(str, tok);
00688                 strcat(str, " ");
00689                 VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00690             }
00691             strcat(str, tok);
00692             strncpy(strnew, str+1, strlen(str)-2);
00693             strcpy(tok, strnew);
00694         }
00695         if (thee->gotparm) {
00696             Vnm_print(2, "Nosh: Hey! You already specified a parameterfile (%s)!\n", thee->parmpath);
00697             Vnm_print(2, "Nosh: I'm going to ignore this one (%s)!\n", tok);
00698         } else {
00699             thee->parmfmt = parmfmt;
00700             thee->gotparm = 1;
00701             strncpy(thee->parmpath, tok, VMAX_ARGLEN);
00702         }
00703     } else if (Vstring_strcasecmp(tok, "xml") == 0) {
00704         parmfmt = NPF_XML;
00705         VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00706         if (tok[0]=='"') {
00707             strcpy(strnew, "");
00708             while (tok[strlen(tok)-1] != '"') {
00709                 strcat(str, tok);
00710                 strcat(str, " ");
00711                 VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00712             }
00713             strcat(str, tok);
00714             strncpy(strnew, str+1, strlen(str)-2);
00715             strcpy(tok, strnew);
00716         }
00717         if (thee->gotparm) {
00718             Vnm_print(2, "Nosh: Hey! You already specified a parameterfile (%s)!\n", thee->parmpath);
00719             Vnm_print(2, "Nosh: I'm going to ignore this one (%s)!\n", tok);
00720         } else {
00721             thee->parmfmt = parmfmt;
00722             thee->gotparm = 1;
00723             strncpy(thee->parmpath, tok, VMAX_ARGLEN);
00724         }
00725     } else {
00726         Vnm_print(2, "Nosh_parseREAD: Ignoring undefined parm format \
00727 %s!\n", tok);
00728     }
00729
00730     return 1;
00731
00732
00733 ERROR1:
00734     Vnm_print(2, "Nosh_parseREAD_PARM: Ran out of tokens while parsing READ section!\n");
00735     return 0;
00736
00737 }
00738

```

```

00739 VPRIVATE int Nosh_parseREAD_DIEL(NOsh *thee, Vio *sock) {
00740
00741     char tok[VMAX_BUFSIZE], str[VMAX_BUFSIZE]="", strnew[VMAX_BUFSIZE]="";
00742     Vdata_Format dielfmt;
00743
00744     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00745     if (Vstring_strcasecmp(tok, "dx") == 0) {
00746         dielfmt = VDF_DX;
00747         //added VDF_BIN to take binary files.
00748     } else if (Vstring_strcasecmp(tok, "dxbin") == 0){
00749         dielfmt = VDF_DXBIN;
00750     } else if (Vstring_strcasecmp(tok, "gz") == 0) {
00751         dielfmt = VDF_GZ;
00752     } else {
00753         Vnm_print(2, "Nosh_parseREAD: Ignoring undefined format \
00754                 %s!\n", tok);
00755         return VRC_FAILURE;
00756     }
00757
00758     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00759     if (tok[0]=='"') {
00760         strcpy(strnew, "");
00761         while (tok[strlen(tok)-1] != '"') {
00762             strcat(str, tok);
00763             strcat(str, " ");
00764             VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00765         }
00766         strcat(str, tok);
00767         strncpy(strnew, str+1, strlen(str)-2);
00768         strcpy(tok, strnew);
00769     }
00770     Vnm_print(0, "Nosh: Storing x-shifted dielectric map %d path \
00771             %s\n", thee->ndiel, tok);
00772     strncpy(thee->dielXpath[thee->ndiel], tok, VMAX_ARGLEN);
00773     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00774     Vnm_print(0, "Nosh: Storing y-shifted dielectric map %d path \
00775             %s\n", thee->ndiel, tok);
00776     strncpy(thee->dielYpath[thee->ndiel], tok, VMAX_ARGLEN);
00777     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00778     Vnm_print(0, "Nosh: Storing z-shifted dielectric map %d path \
00779             %s\n", thee->ndiel, tok);
00780     strncpy(thee->dielZpath[thee->ndiel], tok, VMAX_ARGLEN);
00781     thee->dielfmt[thee->ndiel] = dielfmt;
00782     (thee->ndiel)++;
00783
00784     return 1;
00785
00786 VERROR1:
00787     Vnm_print(2, "Nosh_parseREAD_DIEL: Ran out of tokens while parsing READ \
00788 section!\n");
00789     return 0;
00790
00791 }
00792
00793 VPRIVATE int Nosh_parseREAD_KAPPA(NOsh *thee, Vio *sock) {
00794
00795     char tok[VMAX_BUFSIZE], str[VMAX_BUFSIZE]="", strnew[VMAX_BUFSIZE]="";
00796     Vdata_Format kappafmt;
00797
00798     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00799     if (Vstring_strcasecmp(tok, "dx") == 0) {
00800         kappafmt = VDF_DX;
00801     } else if (Vstring_strcasecmp(tok, "gz") == 0) {
00802         kappafmt = VDF_GZ;
00803     } else if (Vstring_strcasecmp(tok, "dxbin") == 0) {
00804         kappafmt = VDF_DXBIN;
00805     } else {
00806
00807         Vnm_print(2, "Nosh_parseREAD: Ignoring undefined format \
00808                 %s!\n", tok);
00809         return VRC_FAILURE;
00810     }
00811
00812     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00813     if (tok[0]=='"') {
00814         strcpy(strnew, "");
00815         while (tok[strlen(tok)-1] != '"') {
00816             strcat(str, tok);
00817             strcat(str, " ");
00818             VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00819         }

```



```

00820         strcat(str, tok);
00821         strncpy(strnew, str+1, strlen(str)-2);
00822         strcpy(tok, strnew);
00823     }
00824     Vnm_print(0, "Nosh: Storing kappa map %d path %s\n",
00825         thee->nkappa, tok);
00826     thee->kappafmt[thee->nkappa] = kappafmt;
00827     strncpy(thee->kappapath[thee->nkappa], tok, VMAX_ARGLEN);
00828     (thee->nkappa)++;
00829
00830     return 1;
00831
00832 ERROR1:
00833     Vnm_print(2, "Nosh_parseREAD: Ran out of tokens while parsing READ \
00834 section!\n");
00835     return 0;
00836
00837 }
00838
00839 VPRIVATE int Nosh_parseREAD_POTENTIAL(Nosh *thee, Vio *sock) {
00840
00841     char tok[VMAX_BUFSIZE], str[VMAX_BUFSIZE]="", strnew[VMAX_BUFSIZE]="";
00842     Vdata_Format potfmt;
00843
00844     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00845     if (Vstring_strcasecmp(tok, "dx") == 0) {
00846         potfmt = VDF_DX;
00847     } else if (Vstring_strcasecmp(tok, "gz") == 0) {
00848         potfmt = VDF_GZ;
00849     } else if (Vstring_strcasecmp(tok, "dxbin") == 0) {
00850         potfmt = VDF_DXBIN;
00851     } else {
00852         Vnm_print(2, "Nosh_parseREAD: Ignoring undefined format \
00853 %s!\n", tok);
00854         return VRC_FAILURE;
00855     }
00856
00857     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00858     if (tok[0]=='"') {
00859         strcpy(strnew, "");
00860         while (tok[strlen(tok)-1] != '"') {
00861             strcat(str, tok);
00862             strcat(str, " ");
00863             VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00864         }
00865         strcat(str, tok);
00866         strncpy(strnew, str+1, strlen(str)-2);
00867         strcpy(tok, strnew);
00868     }
00869     Vnm_print(0, "Nosh: Storing potential map %d path %s\n",
00870         thee->npot, tok);
00871     thee->potfmt[thee->npot] = potfmt;
00872     strncpy(thee->potpath[thee->npot], tok, VMAX_ARGLEN);
00873     (thee->npot)++;
00874
00875     return 1;
00876
00877 ERROR1:
00878     Vnm_print(2, "Nosh_parseREAD: Ran out of tokens while parsing READ \
00879 section!\n");
00880     return 0;
00881
00882 }
00883
00884 VPRIVATE int Nosh_parseREAD_CHARGE(Nosh *thee, Vio *sock) {
00885
00886     char tok[VMAX_BUFSIZE], str[VMAX_BUFSIZE]="", strnew[VMAX_BUFSIZE]="";
00887     Vdata_Format chargefmt;
00888
00889     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00890     if (Vstring_strcasecmp(tok, "dx") == 0) {
00891         chargefmt = VDF_DX;
00892     }
00893     else if (Vstring_strcasecmp(tok, "dxbin") == 0) {
00894         chargefmt = VDF_DXBIN;
00895     } else if (Vstring_strcasecmp(tok, "gz") == 0) {
00896         chargefmt = VDF_GZ;
00897     } else {
00898         Vnm_print(2, "Nosh_parseREAD: Ignoring undefined format \
00899 %s!\n", tok);
00900         return VRC_FAILURE;

```

```

00901     }
00902
00903     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00904     if (tok[0]!=' ') {
00905         strcpy(strnew, "");
00906         while (tok[strlen(tok)-1] != ' ') {
00907             strcat(str, tok);
00908             strcat(str, " ");
00909             VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00910         }
00911         strcat(str, tok);
00912         strncpy(strnew, str+1, strlen(str)-2);
00913         strcpy(tok, strnew);
00914     }
00915     Vnm_print(0, "Nosh: Storing charge map %d path %s\n",
00916             thee->ncharge, tok);
00917     thee->chargefmt[thee->ncharge] = chargefmt;
00918     strncpy(thee->chargepath[thee->ncharge], tok, VMAX_ARGLEN);
00919     (thee->ncharge)++;
00920
00921     return 1;
00922
00923 VERROR1:
00924     Vnm_print(2, "Nosh_parseREAD: Ran out of tokens while parsing READ \
00925 section!\n");
00926     return 0;
00927
00928 }
00929
00930 VPRIVATE int Nosh_parseREAD_MESH(Nosh *thee, Vio *sock) {
00931
00932     char tok[VMAX_BUFSIZE], str[VMAX_BUFSIZE]="", strnew[VMAX_BUFSIZE]="";
00933     Vdata_Format meshfmt;
00934
00935     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00936     if (Vstring_strcasecmp(tok, "mcsf") == 0) {
00937         meshfmt = VDF_MCSF;
00938         VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00939         if (tok[0]!=' ') {
00940             strcpy(strnew, "");
00941             while (tok[strlen(tok)-1] != ' ') {
00942                 strcat(str, tok);
00943                 strcat(str, " ");
00944                 VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00945             }
00946             strcat(str, tok);
00947             strncpy(strnew, str+1, strlen(str)-2);
00948             strcpy(tok, strnew);
00949         }
00950         Vnm_print(0, "Nosh: Storing mesh %d path %s\n",
00951             thee->nmesh, tok);
00952         thee->meshfmt[thee->nmesh] = meshfmt;
00953         strncpy(thee->meshpath[thee->nmesh], tok, VMAX_ARGLEN);
00954         (thee->nmesh)++;
00955     } else {
00956         Vnm_print(2, "Nosh_parseREAD: Ignoring undefined mesh format \
00957 %s!\n", tok);
00958     }
00959
00960     return 1;
00961
00962 VERROR1:
00963     Vnm_print(2, "Nosh_parseREAD: Ran out of tokens while parsing READ \
00964 section!\n");
00965     return 0;
00966
00967 }
00968
00969
00970 VPRIVATE int Nosh_parseREAD(Nosh *thee, Vio *sock) {
00971
00972     char tok[VMAX_BUFSIZE];
00973
00974     if (thee == VNULL) {
00975         Vnm_print(2, "Nosh_parseREAD: Got NULL thee!\n");
00976         return 0;
00977     }
00978
00979     if (sock == VNULL) {
00980         Vnm_print(2, "Nosh_parseREAD: Got pointer to NULL socket!\n");
00981         return 0;

```

```

00982     }
00983
00984     if (thee->parsed) {
00985         Vnm_print(2, "Nosh_parseREAD:  Already parsed an input file!\n");
00986         return 0;
00987     }
00988
00989     /* Read until we run out of tokens (bad) or hit the "END" keyword (good) */
00990     while (Vio_scanf(sock, "%s", tok) == 1) {
00991         if (Vstring_strcasecmp(tok, "end") == 0) {
00992             Vnm_print(0, "Nosh: Done parsing READ section\n");
00993             return 1;
00994         } else if (Vstring_strcasecmp(tok, "mol") == 0) {
00995             Nosh_parseREAD_MOL(thee, sock);
00996         } else if (Vstring_strcasecmp(tok, "parm") == 0) {
00997             Nosh_parseREAD_PARM(thee, sock);
00998         } else if (Vstring_strcasecmp(tok, "diel") == 0) {
00999             Nosh_parseREAD_DIEL(thee, sock);
01000         } else if (Vstring_strcasecmp(tok, "kappa") == 0) {
01001             Nosh_parseREAD_KAPPA(thee, sock);
01002         } else if (Vstring_strcasecmp(tok, "pot") == 0) {
01003             Nosh_parseREAD_POTENTIAL(thee, sock);
01004         } else if (Vstring_strcasecmp(tok, "charge") == 0) {
01005             Nosh_parseREAD_CHARGE(thee, sock);
01006         } else if (Vstring_strcasecmp(tok, "mesh") == 0) {
01007             Nosh_parseREAD_MESH(thee, sock);
01008         } else {
01009             Vnm_print(2, "Nosh_parseREAD:  Ignoring undefined keyword %s!\n",
01010                     tok);
01011         }
01012     }
01013
01014     /* We ran out of tokens! */
01015     Vnm_print(2, "Nosh_parseREAD:  Ran out of tokens while parsing READ \
01016 section!\n");
01017     return 0;
01018 }
01019
01020 VPRIVATE int Nosh_parsePRINT(NOsh *thee, Vio *sock) {
01021     char tok[VMAX_BUFSIZE];
01022     char name[VMAX_BUFSIZE];
01023     int ti, idx, expect, ielec, iapol;
01024
01025     if (thee == VNULL) {
01026         Vnm_print(2, "Nosh_parsePRINT:  Got NULL thee!\n");
01027         return 0;
01028     }
01029
01030     if (sock == VNULL) {
01031         Vnm_print(2, "Nosh_parsePRINT:  Got pointer to NULL socket!\n");
01032         return 0;
01033     }
01034
01035     if (thee->parsed) {
01036         Vnm_print(2, "Nosh_parsePRINT:  Already parsed an input file!\n");
01037         return 0;
01038     }
01039
01040     idx = thee->nprint;
01041     if (thee->nprint >= NOSH_MAXPRINT) {
01042         Vnm_print(2, "Nosh_parsePRINT:  Exceeded max number (%d) of PRINT \
01043 sections\n",
01044                 NOSH_MAXPRINT);
01045         return 0;
01046     }
01047
01048     /* The first thing we read is the thing we want to print */
01049     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
01050     if (Vstring_strcasecmp(tok, "energy") == 0) {
01051         thee->printwhat[idx] = NPT_ENERGY;
01052         thee->printnarg[idx] = 0;
01053     } else if (Vstring_strcasecmp(tok, "force") == 0) {
01054         thee->printwhat[idx] = NPT_FORCE;
01055         thee->printnarg[idx] = 0;
01056     } else if (Vstring_strcasecmp(tok, "elecEnergy") == 0) {
01057         thee->printwhat[idx] = NPT_ELECENERGY;
01058         thee->printnarg[idx] = 0;
01059     } else if (Vstring_strcasecmp(tok, "elecForce") == 0) {

```

```

01063     thee->printwhat[idx] = NPT_ELECFORCE;
01064     thee->printnarg[idx] = 0;
01065     } else if (Vstring_strcasecmp(tok, "apolEnergy") == 0) {
01066         thee->printwhat[idx] = NPT_APOLENERGY;
01067         thee->printnarg[idx] = 0;
01068     } else if (Vstring_strcasecmp(tok, "apolForce") == 0) {
01069         thee->printwhat[idx] = NPT_APOLFORCE;
01070         thee->printnarg[idx] = 0;
01071     } else {
01072         Vnm_print(2, "Nosh_parsePRINT: Undefined keyword %s while parsing \
01073 PRINT section!\n", tok);
01074         return 0;
01075     }
01076
01077     expect = 0; /* We first expect a calculation ID (0) then an op (1) */
01078
01079     /* Read until we run out of tokens (bad) or hit the "END" keyword (good) */
01080     while (Vio_scanf(sock, "%s", tok) == 1) {
01081
01082         /* The next thing we read is either END or an ARG OP ARG statement */
01083         if (Vstring_strcasecmp(tok, "end") == 0) {
01084             if (expect != 0) {
01085                 (thee->nprint)++;
01086                 (thee->printnarg[idx])++;
01087                 Vnm_print(0, "Nosh: Done parsing PRINT section\n");
01088                 return 1;
01089             } else {
01090                 Vnm_print(2, "Nosh_parsePRINT: Got premature END to PRINT!\n");
01091                 return 0;
01092             }
01093         } else {
01094
01095             /* Grab a calculation ID */
01096             if ((sscanf(tok, "%d", &ti) == 1) &&
01097                 (Vstring_isdigit(tok) == 1)) {
01098                 if (expect == 0) {
01099                     thee->printcalc[idx][thee->printnarg[idx]] = ti-1;
01100                     expect = 1;
01101                 } else {
01102                     Vnm_print(2, "Nosh_parsePRINT: Syntax error in PRINT \
01103 section while reading %s!\n", tok);
01104                     return 0;
01105                 }
01106                 /* Grab addition operation */
01107                 } else if (Vstring_strcasecmp(tok, "+") == 0) {
01108                     if (expect == 1) {
01109                         thee->printop[idx][thee->printnarg[idx]] = 0;
01110                         (thee->printnarg[idx])++;
01111                         expect = 0;
01112                         if (thee->printnarg[idx] >= NOSH_MAXPOP) {
01113                             Vnm_print(2, "Nosh_parsePRINT: Exceeded max number \
01114 (%d) of arguments for PRINT section!\n",
01115                                     NOSH_MAXPOP);
01116                             return 0;
01117                         }
01118                     } else {
01119                         Vnm_print(2, "Nosh_parsePRINT: Syntax error in PRINT \
01120 section while reading %s!\n", tok);
01121                         return 0;
01122                     }
01123                 /* Grab subtraction operation */
01124                 } else if (Vstring_strcasecmp(tok, "-") == 0) {
01125                     if (expect == 1) {
01126                         thee->printop[idx][thee->printnarg[idx]] = 1;
01127                         (thee->printnarg[idx])++;
01128                         expect = 0;
01129                         if (thee->printnarg[idx] >= NOSH_MAXPOP) {
01130                             Vnm_print(2, "Nosh_parsePRINT: Exceeded max number \
01131 (%d) of arguments for PRINT section!\n",
01132                                     NOSH_MAXPOP);
01133                             return 0;
01134                         }
01135                     } else {
01136                         Vnm_print(2, "Nosh_parsePRINT: Syntax error in PRINT \
01137 section while reading %s!\n", tok);
01138                         return 0;
01139                     }
01140                 /* Grab a calculation name from elec ID */
01141                 } else if (sscanf(tok, "%s", name) == 1) {
01142                     if (expect == 0) {
01143                         for (ielec=0; ielec<thee->nelec; ielec++) {

```

```

01144         if (Vstring_strcasecmp(thee->elecname[ielec], name) == 0) {
01145             thee->printcalc[idx][thee->printnarg[idx]] = ielec;
01146             expect = 1;
01147             break;
01148         }
01149     }
01150     for (iapol=0; iapol<thee->napol; iapol++) {
01151         if (Vstring_strcasecmp(thee->apolname[iapol], name) == 0) {
01152             thee->printcalc[idx][thee->printnarg[idx]] = iapol;
01153             expect = 1;
01154             break;
01155         }
01156     }
01157     if (expect == 0) {
01158         Vnm_print(2, "No ELEC or APOL statement has been named %s!\n",
01159                 name);
01160         return 0;
01161     }
01162     } else {
01163         Vnm_print(2, "Nosh_parsePRINT: Syntax error in PRINT \
01164 section while reading %s!\n", tok);
01165         return 0;
01166     }
01167     /* Got bad operation */
01168     } else {
01169         Vnm_print(2, "Nosh_parsePRINT: Undefined keyword %s while \
01170 parsing PRINT section!\n", tok);
01171         return 0;
01172     }
01173     } /* end parse token */
01174 } /* end while */
01175 } /* We ran out of tokens! */
01176
01177 VJMPERR1(0);
01178
01179 /* We ran out of tokens! */
01180 ERROR1:
01181     Vnm_print(2, "Nosh_parsePRINT: Ran out of tokens while parsing PRINT \
01182 section!\n");
01183     return 0;
01184 }
01185 }
01186
01187 VPRIVATE int Nosh_parseELEC(Nosh *thee, Vio *sock) {
01188     Nosh_calc *calc = VNULL;
01189     char tok[VMAX_BUFSIZE];
01190
01191     if (thee == VNULL) {
01192         Vnm_print(2, "Nosh_parseELEC: Got NULL thee!\n");
01193         return 0;
01194     }
01195     if (sock == VNULL) {
01196         Vnm_print(2, "Nosh_parseELEC: Got pointer to NULL socket!\n");
01197         return 0;
01198     }
01199     if (thee->parsed) {
01200         Vnm_print(2, "Nosh_parseELEC: Already parsed an input file!\n");
01201         return 0;
01202     }
01203     /* Get a pointer to the latest ELEC calc object and update the ELEC
01204 statement number */
01205     if (thee->nelec >= NOSH_MAXCALC) {
01206         Vnm_print(2, "Nosh: Too many electrostatics calculations in this \
01207 run!\n");
01208         Vnm_print(2, "Nosh: Current max is %d; ignoring this calculation\n",
01209                 NOSH_MAXCALC);
01210         return 1;
01211     }
01212     /* The next token HAS to be the method OR "name" */
01213     if (Vio_scanf(sock, "%s", tok) == 1) {
01214         if (Vstring_strcasecmp(tok, "name") == 0) {
01215             Vio_scanf(sock, "%s", tok);
01216             strncpy(thee->elecname[thee->nelec], tok, VMAX_ARGLEN);
01217             if (Vio_scanf(sock, "%s", tok) != 1) {
01218                 Vnm_print(2, "Nosh_parseELEC: Ran out of tokens while reading \

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```

01225 ELEC section!\n");
01226         return 0;
01227     }
01228 }
01229 if (Vstring_strcasecmp(tok, "mg-manual") == 0) {
01230     thee->elec[thee->nelec] = Nosh_calc_ctor(NCT_MG);
01231     calc = thee->elec[thee->nelec];
01232     (thee->nelec)++;
01233     calc->mgparm->type = MCT_MANUAL;
01234     return Nosh_parseMG(thee, sock, calc);
01235 } else if (Vstring_strcasecmp(tok, "mg-auto") == 0) {
01236     thee->elec[thee->nelec] = Nosh_calc_ctor(NCT_MG);
01237     calc = thee->elec[thee->nelec];
01238     (thee->nelec)++;
01239     calc->mgparm->type = MCT_AUTO;
01240     return Nosh_parseMG(thee, sock, calc);
01241 } else if (Vstring_strcasecmp(tok, "mg-para") == 0) {
01242     thee->elec[thee->nelec] = Nosh_calc_ctor(NCT_MG);
01243     calc = thee->elec[thee->nelec];
01244     (thee->nelec)++;
01245     calc->mgparm->type = MCT_PARALLEL;
01246     return Nosh_parseMG(thee, sock, calc);
01247 } else if (Vstring_strcasecmp(tok, "mg-dummy") == 0) {
01248     thee->elec[thee->nelec] = Nosh_calc_ctor(NCT_MG);
01249     calc = thee->elec[thee->nelec];
01250     (thee->nelec)++;
01251     calc->mgparm->type = MCT_DUMMY;
01252     return Nosh_parseMG(thee, sock, calc);
01253 } else if (Vstring_strcasecmp(tok, "fe-manual") == 0) {
01254     thee->elec[thee->nelec] = Nosh_calc_ctor(NCT_FEM);
01255     calc = thee->elec[thee->nelec];
01256     (thee->nelec)++;
01257     calc->femparm->type = FCT_MANUAL;
01258     return Nosh_parseFEM(thee, sock, calc);
01259 } else if (Vstring_strcasecmp(tok, "tabi") == 0) {
01260     thee->elec[thee->nelec] = Nosh_calc_ctor(NCT_BEM);
01261     calc = thee->elec[thee->nelec];
01262     (thee->nelec)++;
01263     calc->bemparm->type = BCT_MANUAL;
01264     return Nosh_parseBEM(thee, sock, calc);
01265 } else if (Vstring_strcasecmp(tok, "bem") == 0) {
01266     thee->elec[thee->nelec] = Nosh_calc_ctor(NCT_BEM);
01267     calc = thee->elec[thee->nelec];
01268     (thee->nelec)++;
01269     calc->bemparm->type = BCT_MANUAL;
01270     return Nosh_parseBEM(thee, sock, calc);
01271 } else if (Vstring_strcasecmp(tok, "bem-manual") == 0) {
01272     thee->elec[thee->nelec] = Nosh_calc_ctor(NCT_BEM);
01273     calc = thee->elec[thee->nelec];
01274     (thee->nelec)++;
01275     calc->bemparm->type = BCT_MANUAL;
01276     return Nosh_parseBEM(thee, sock, calc);
01277 } else if (Vstring_strcasecmp(tok, "geoflow-manual") == 0) {
01278     Vnm_print(2, "Geoflow currently does not support geoflow-manual please use geoflow instead!\n");
01279     return 0;
01280 } else if (Vstring_strcasecmp(tok, "geoflow-none") == 0) {
01281     Vnm_print(2, "Geoflow currently does not support geoflow-none please use geoflow instead!\n");
01282     return 0;
01283 } else if (Vstring_strcasecmp(tok, "geoflow") == 0) {
01284     thee->elec[thee->nelec] = Nosh_calc_ctor(NCT_GEOFLOW);
01285     calc = thee->elec[thee->nelec];
01286     (thee->nelec)++;
01287     calc->geoflowparm->type = GFCT_AUTO;
01288     return Nosh_parseGEOFLOW(thee, sock, calc);
01289 } else if (Vstring_strcasecmp(tok, "pbam") == 0) {
01290     thee->elec[thee->nelec] = Nosh_calc_ctor(NCT_PBAM);
01291     calc = thee->elec[thee->nelec];
01292     (thee->nelec)++;
01293     calc->pbamparm->type = PBAMCT_AUTO;
01294     return Nosh_parsePBAM(thee, sock, calc);
01295 } else if (Vstring_strcasecmp(tok, "pbsam") == 0) {
01296     thee->elec[thee->nelec] = Nosh_calc_ctor(NCT_PBSAM);
01297     calc = thee->elec[thee->nelec];
01298     (thee->nelec)++;
01299     calc->pbsamparm->type = PBSAMCT_AUTO;
01300     return Nosh_parsePBSAM(thee, sock, calc);
01301 } else {
01302     Vnm_print(2, "Nosh_parseELEC: The method (\\"mg\\", \\"fem\\", \\"bem\\", \\"geoflow\\", \\"pbam\\",
01303     \\"pbsam\\") or \\"name\\" must be the first keyword in the ELEC section\n");
01304     return 0;

```

```

01305     }
01306 }
01307
01308 Vnm_print(2, "Nosh_parseELEC: Ran out of tokens while reading ELEC section!\n");
01309 return 0;
01310
01311 }
01312
01313 VPRIVATE int Nosh_parseAPOLAR(NOsh *thee, Vio *sock) {
01314     NOsh_calc *calc = VNULL;
01315
01316     char tok[VMAX_BUFSIZE];
01317
01318     if (thee == VNULL) {
01319         Vnm_print(2, "Nosh_parseAPOLAR: Got NULL thee!\n");
01320         return 0;
01321     }
01322
01323     if (sock == VNULL) {
01324         Vnm_print(2, "Nosh_parseAPOLAR: Got pointer to NULL socket!\n");
01325         return 0;
01326     }
01327
01328     if (thee->parsed) {
01329         Vnm_print(2, "Nosh_parseAPOLAR: Already parsed an input file!\n");
01330         return 0;
01331     }
01332
01333     /* Get a pointer to the latest ELEC calc object and update the ELEC
01334        statement number */
01335     if (thee->napol >= NOSH_MAXCALC) {
01336         Vnm_print(2, "Nosh: Too many non-polar calculations in this \
01337 run!\n");
01338         Vnm_print(2, "Nosh: Current max is %d; ignoring this calculation\n",
01339                 NOSH_MAXCALC);
01340         return 1;
01341     }
01342
01343     /* The next token HAS to be the method OR "name" */
01344     if (Vio_scanf(sock, "%s", tok) == 1) {
01345         if (Vstring_strcasecmp(tok, "name") == 0) {
01346             Vio_scanf(sock, "%s", tok);
01347             strncpy(thee->apolname[thee->napol], tok, VMAX_ARGLEN);
01348
01349             /* Parse the non-polar parameters */
01350             thee->apol[thee->napol] = Nosh_calc_ctor(NCT_APOL);
01351             calc = thee->apol[thee->napol];
01352             (thee->napol)++;
01353             return Nosh_parseAPOL(thee, sock, calc);
01354         } else if (Vstring_strcasecmp(tok, "geoflow-manual") == 0) {
01355             thee->elec[thee->nelec] = Nosh_calc_ctor(NCT_GEOFLOW);
01356             calc = thee->elec[thee->nelec];
01357             (thee->nelec)++;
01358             calc->geoflowparm->type = GFCT_MANUAL;
01359             return Nosh_parseGEOFLOW(thee, sock, calc);
01360         } else if (Vstring_strcasecmp(tok, "geoflow-auto") == 0) {
01361             thee->elec[thee->nelec] = Nosh_calc_ctor(NCT_GEOFLOW);
01362             calc = thee->elec[thee->nelec];
01363             (thee->nelec)++;
01364             calc->geoflowparm->type = GFCT_AUTO;
01365             return Nosh_parseGEOFLOW(thee, sock, calc);
01366         }
01367     }
01368 }
01369
01370 return 1;
01371
01372 }
01373
01374 VPUBLIC int Nosh_setupElecCalc(
01375     NOsh *thee,
01376     Valist *alist[NOSH_MAXMOL]
01377 ) {
01378     int ielec, imol, i;
01379     NOsh_calc *elec = VNULL;
01380     MGparm *mgparm = VNULL;
01381     Valist *mymol = VNULL;
01382
01383     VASSERT(thee != VNULL);
01384     for (imol=0; imol<thee->nmol; imol++) {
01385         thee->alist[imol] = alist[imol];

```

```

01386     }
01387
01388
01389     for (ielec=0; ielec<(thee->nelec); ielec++) {
01390         /* Unload the calculation object containing the ELEC information */
01391         elec = thee->elec[ielec];
01392
01393         if (((thee->ndiel != 0) || (thee->nkappa != 0) ||
01394             (thee->ncharge != 0) || (thee->npot != 0)) &&
01395             (elec->pbeparm->calcforce != PCF_NO)) {
01396             Vnm_print(2, "Nosh_setupElecCalc: Calculation of forces disabled because surface \
01397 map is used!\n");
01398             elec->pbeparm->calcforce = PCF_NO;
01399         }
01400
01401         /* Setup the calculation */
01402         switch (elec->calctype) {
01403             case NCT_MG:
01404                 /* Center on the molecules, if requested */
01405                 mgparm = elec->mgparm;
01406                 VASSERT(mgparm != VNULL);
01407                 if (elec->mgparm->cmeth == MCM_MOLECULE) {
01408                     VASSERT(mgparm->centmol >= 0);
01409                     VASSERT(mgparm->centmol < thee->nmol);
01410                     mymol = thee->alist[mgparm->centmol];
01411                     VASSERT(mymol != VNULL);
01412                     for (i=0; i<3; i++) {
01413                         mgparm->center[i] = mymol->center[i];
01414                     }
01415                 }
01416                 if (elec->mgparm->fcmeth == MCM_MOLECULE) {
01417                     VASSERT(mgparm->fcentmol >= 0);
01418                     VASSERT(mgparm->fcentmol < thee->nmol);
01419                     mymol = thee->alist[mgparm->fcentmol];
01420                     VASSERT(mymol != VNULL);
01421                     for (i=0; i<3; i++) {
01422                         mgparm->fcenter[i] = mymol->center[i];
01423                     }
01424                 }
01425                 if (elec->mgparm->ccmeth == MCM_MOLECULE) {
01426                     VASSERT(mgparm->ccentmol >= 0);
01427                     VASSERT(mgparm->ccentmol < thee->nmol);
01428                     mymol = thee->alist[mgparm->ccentmol];
01429                     VASSERT(mymol != VNULL);
01430                     for (i=0; i<3; i++) {
01431                         mgparm->ccenter[i] = mymol->center[i];
01432                     }
01433                 }
01434                 Nosh_setupCalcMG(thee, elec);
01435                 break;
01436             case NCT_FEM:
01437                 Nosh_setupCalcFEM(thee, elec);
01438                 break;
01439             case NCT_PBAM:
01440                 Nosh_setupCalcPBAM(thee, elec);
01441                 break;
01442             case NCT_PBSAM:
01443                 Nosh_setupCalcPBSAM(thee, elec);
01444                 break;
01445             case NCT_BEM:
01446                 Nosh_setupCalcBEM(thee, elec);
01447                 break;
01448             case NCT_GEOFLOW:
01449                 Nosh_setupCalcGEOFLOW(thee, elec);
01450                 break;
01451             default:
01452                 Vnm_print(2, "Nosh_setupCalc: Invalid calculation type (%d)!\n",
01453                     elec->calctype);
01454                 return 0;
01455         }
01456
01457         /* At this point, the most recently-created Nosh_calc object should be the
01458            one we use for results for this ELEC statement. Assign it. */
01459         /* Associate ELEC statement with the calculation */
01460         thee->elec2calc[ielec] = thee->ncalc-1;
01461         Vnm_print(0, "Nosh_setupCalc: Mapping ELEC statement %d (%d) to \
01462 calculation %d (%d)\n", ielec, ielec+1, thee->elec2calc[ielec],
01463             thee->elec2calc[ielec]+1);
01464     }
01465
01466     return 1;

```



```

01467 }
01468
01469 VPUBLIC int NOsh_setupApolCalc(
01470     NOsh *thee,
01471     Valist *alist[NOSH_MAXMOL]
01472 ) {
01473     int iapol, imol;
01474     int doCalc = ACD_NO;
01475     NOsh_calc *calc = VNULL;
01476
01477     VASSERT(thee != VNULL);
01478     for (imol=0; imol<thee->nmol; imol++) {
01479         thee->alist[imol] = alist[imol];
01480     }
01481
01482     for (iapol=0; iapol<(thee->napol); iapol++) {
01483         /* Unload the calculation object containing the APOL information */
01484         calc = thee->apol[iapol];
01485
01486         /* Setup the calculation */
01487         switch (calc->calctype) {
01488             case NCT_APOL:
01489                 NOsh_setupCalcAPOL(thee, calc);
01490                 doCalc = ACD_YES;
01491                 break;
01492             default:
01493                 Vnm_print(2, "NOsh_setupCalc: Invalid calculation type (%d)!\n", calc->calctype);
01494                 return ACD_ERROR;
01495         }
01496         /* At this point, the most recently-created NOsh_calc object should be the
01497            one we use for results for this APOL statement. Assign it. */
01498         /* Associate APOL statement with the calculation */
01499         thee->apol2calc[iapol] = thee->ncalc-1;
01500         Vnm_print(0, "NOsh_setupCalc: Mapping APOL statement %d (%d) to calculation %d (%d)\n", iapol,
01501             iapol+1, thee->apol2calc[iapol], thee->apol2calc[iapol]+1);
01502     }
01503
01504     if (doCalc == ACD_YES) {
01505         return ACD_YES;
01506     } else {
01507         return ACD_NO;
01508     }
01509 }
01510
01510 VPUBLIC int NOsh_parseMG(
01511     NOsh *thee,
01512     Vio *sock,
01513     NOsh_calc *elec
01514 ) {
01515     char tok[VMAX_BUFSIZE];
01516     MGparm *mgparm = VNULL;
01517     PBEParm *pbeparm = VNULL;
01518     int rc;
01519
01520     /* Check the arguments */
01521     if (thee == VNULL) {
01522         Vnm_print(2, "NOsh: Got NULL thee!\n");
01523         return 0;
01524     }
01525
01526     if (sock == VNULL) {
01527         Vnm_print(2, "NOsh: Got pointer to NULL socket!\n");
01528         return 0;
01529     }
01530
01531     if (elec == VNULL) {
01532         Vnm_print(2, "NOsh: Got pointer to NULL elec object!\n");
01533         return 0;
01534     }
01535
01536     mgparm = elec->mgparm;
01537     if (mgparm == VNULL) {
01538         Vnm_print(2, "NOsh: Got pointer to NULL mgparm object!\n");
01539         return 0;
01540     }
01541
01542     pbeparm = elec->pbeparm;
01543     if (pbeparm == VNULL) {
01544         Vnm_print(2, "NOsh: Got pointer to NULL pbeparm object!\n");
01545         return 0;
01546     }
01547
01548     Vnm_print(0, "NOsh_parseMG: Parsing parameters for MG calculation\n");
01549 }

```

```

01547     /* Parallel stuff */
01548     if (mgparm->type == MCT_PARALLEL) {
01549         mgparm->proc_rank = thee->proc_rank;
01550         mgparm->proc_size = thee->proc_size;
01551         mgparm->setrank = 1;
01552         mgparm->setsize = 1;
01553     }
01554
01555
01556     /* Start snarfing tokens from the input stream */
01557     rc = 1;
01558     while (Vio_scanf(sock, "%s", tok) == 1) {
01559
01560         Vnm_print(0, "Nosh_parseMG: Parsing %s...\n", tok);
01561
01562         /* See if it's an END token */
01563         if (Vstring_strcasecmp(tok, "end") == 0) {
01564             mgparm->parsed = 1;
01565             pbeparm->parsed = 1;
01566             rc = 1;
01567             break;
01568         }
01569
01570         /* Pass the token through a series of parsers */
01571         rc = PBEParm_parseToken(pbeparm, tok, sock);
01572         if (rc == -1) {
01573             Vnm_print(0, "Nosh_parseMG: parsePBE error!\n");
01574             break;
01575         } else if (rc == 0) {
01576             /* Pass the token to the generic MG parser */
01577             rc = MGparm_parseToken(mgparm, tok, sock);
01578             if (rc == -1) {
01579                 Vnm_print(0, "Nosh_parseMG: parseMG error!\n");
01580                 break;
01581             } else if (rc == 0) {
01582                 /* We ran out of parsers! */
01583                 Vnm_print(2, "Nosh: Unrecognized keyword: %s\n", tok);
01584                 break;
01585             }
01586         }
01587     }
01588
01589     /* Handle various errors arising in the token-snarfing loop -- these all
01590        just result in simple returns right now */
01591     if (rc == -1) return 0;
01592     if (rc == 0) return 0;
01593
01594     /* Check the status of the parameter objects */
01595     if ((MGparm_check(mgparm) == VRC_FAILURE) || (!PBEParm_check(pbeparm))) {
01596         Vnm_print(2, "Nosh: MG parameters not set correctly!\n");
01597         return 0;
01598     }
01599
01600     return 1;
01601 }
01602
01603 VPRIVATE int Nosh_setupCalcMG(
01604     Nosh *thee,
01605     Nosh_calc *calc
01606 ) {
01607
01608     MGparm *mgparm = VNULL;
01609
01610     VASSERT(thee != VNULL);
01611     VASSERT(calc != VNULL);
01612     mgparm = calc->mgparm;
01613     VASSERT(mgparm != VNULL);
01614
01615
01616     /* Now we're ready to whatever sorts of post-processing operations that are
01617        necessary for the various types of calculations */
01618     switch (mgparm->type) {
01619         case MCT_MANUAL:
01620             return Nosh_setupCalcMGMANUAL(thee, calc);
01621         case MCT_DUMMY:
01622             return Nosh_setupCalcMGMANUAL(thee, calc);
01623         case MCT_AUTO:
01624             return Nosh_setupCalcMGAUTO(thee, calc);
01625         case MCT_PARALLEL:
01626             return Nosh_setupCalcMGPARA(thee, calc);
01627         default:

```

```

01628         Vnm_print(2, "Nosh_setupCalcMG: undefined MG calculation type (%d)!\n",
01629                     mgparm->type);
01630         return 0;
01631     }
01632
01633     /* Shouldn't get here */
01634     return 0;
01635 }
01636
01637
01638 VPRIVATE int Nosh_setupCalcBEM(
01639     Nosh *thee,
01640     Nosh_calc *calc
01641 ) {
01642
01643     BEMparm *bemparm = VNULL;
01644
01645     VASSERT(thee != VNULL);
01646     VASSERT(calc != VNULL);
01647     bemparm = calc->bemparm;
01648     VASSERT(bemparm != VNULL);
01649
01650
01651     /* Now we're ready to whatever sorts of post-processing operations that are
01652        necessary for the various types of calculations */
01653     switch (bemparm->type) {
01654         case BCT_MANUAL:
01655             return Nosh_setupCalcBEMMANUAL(thee, calc);
01656         default:
01657             Vnm_print(2, "Nosh_setupCalcBEM: undefined BEM calculation type (%d)!\n",
01658                     bemparm->type);
01659             return 0;
01660     }
01661
01662     /* Shouldn't get here */
01663     return 0;
01664 }
01665
01666 VPRIVATE int Nosh_setupCalcGEOFLOW(Nosh *thee, Nosh_calc *calc) {
01667
01668     GEOFLOWparm *parm = VNULL;
01669
01670     VASSERT(thee != VNULL);
01671     VASSERT(calc != VNULL);
01672     parm = calc->geoflowparm;
01673     VASSERT(parm != VNULL);
01674
01675
01676     /* Now we're ready to whatever sorts of post-processing operations that are
01677        necessary for the various types of calculations */
01678     if (/*parm->type == GFCT_MANUAL ||*/ parm->type == GFCT_AUTO) {
01679         return Nosh_setupCalcGEOFLOWMANUAL(thee, calc);
01680     } else {
01681         Vnm_print(2, "Nosh_setupCalcGEOFLOW: undefined GEOFLOW calculation type (%d)!\n", parm->type);
01682         return 0;
01683     }
01684 }
01685
01686 VPRIVATE int Nosh_setupCalcPBAM(Nosh *thee, Nosh_calc *calc) {
01687
01688     PBAMparm *parm = VNULL;
01689
01690     VASSERT(thee != VNULL);
01691     VASSERT(calc != VNULL);
01692     parm = calc->pbamparm;
01693     VASSERT(parm != VNULL);
01694
01695     if (parm->type == PBAMCT_AUTO) {
01696         return Nosh_setupCalcPBAMAUTO(thee, calc);
01697     } else {
01698         Vnm_print(2, "Nosh_setupCalcPBAM: undefined PBAM calculation type (%d)!\n", parm->type);
01699         return 0;
01700     }
01701 }
01702
01703
01704 VPRIVATE int Nosh_setupCalcPBSAM(Nosh *thee, Nosh_calc *calc) {
01705
01706     PBSAMparm *parm = VNULL;
01707
01708     VASSERT(thee != VNULL);

```

```

01709  VASSERT(calc!=VNULL);
01710  parm = calc->pbsamparm;
01711  VASSERT(parm!=VNULL);
01712
01713  if(parm->type == PBSAMCT_AUTO){
01714      return Nosh_setupCalcPBSAMAUTO(thee, calc);
01715  } else {
01716      Vnm_print(2, "Nosh_setupCalcPBSAM: undefined PBSAM calculation type (%d)!\n", parm->type);
01717      return 0;
01718  }
01719 }
01720
01721
01722 VPRIVATE int Nosh_setupCalcFEM(
01723     Nosh *thee,
01724     Nosh_calc *calc
01725 ) {
01726
01727     VASSERT(thee != VNULL);
01728     VASSERT(calc != VNULL);
01729     VASSERT(calc->femparm != VNULL);
01730
01731     /* Now we're ready to whatever sorts of post-processing operations that are
01732      * necessary for the various types of calculations */
01733     switch (calc->femparm->type) {
01734         case FCT_MANUAL:
01735             return Nosh_setupCalcFEMANUAL(thee, calc);
01736         default:
01737             Vnm_print(2, "Nosh_parseFEM: unknown calculation type (%d)!\n",
01738                 calc->femparm->type);
01739             return 0;
01740     }
01741
01742     /* Shouldn't get here */
01743     return 0;
01744 }
01745
01746
01747 VPRIVATE int Nosh_setupCalcMGMANUAL(
01748     Nosh *thee,
01749     Nosh_calc *elec
01750 ) {
01751
01752     MGparm *mgparm = VNULL;
01753     PBEParm *pbeparm = VNULL;
01754     Nosh_calc *calc = VNULL;
01755
01756     if (thee == VNULL) {
01757         Vnm_print(2, "Nosh_setupCalcMGMANUAL: Got NULL thee!\n");
01758         return 0;
01759     }
01760     if (elec == VNULL) {
01761         Vnm_print(2, "Nosh_setupCalcMGMANUAL: Got NULL calc!\n");
01762         return 0;
01763     }
01764     mgparm = elec->mgparm;
01765     if (mgparm == VNULL) {
01766         Vnm_print(2, "Nosh_setupCalcMGMANUAL: Got NULL mgparm -- was this calculation \
01767 set up?\n");
01768         return 0;
01769     }
01770     pbeparm = elec->pbeparm;
01771     if (pbeparm == VNULL) {
01772         Vnm_print(2, "Nosh_setupCalcMGMANUAL: Got NULL pbeparm -- was this calculation \
01773 set up?\n");
01774         return 0;
01775     }
01776
01777     /* Set up missing MG parameters */
01778     if (mgparm->setgrid == 0) {
01779         VASSERT(mgparm->setglen);
01780         mgparm->grid[0] = mgparm->glen[0]/((double) (mgparm->dime[0]-1));
01781         mgparm->grid[1] = mgparm->glen[1]/((double) (mgparm->dime[1]-1));
01782         mgparm->grid[2] = mgparm->glen[2]/((double) (mgparm->dime[2]-1));
01783     }
01784     if (mgparm->setglen == 0) {
01785         VASSERT(mgparm->setgrid);
01786         mgparm->glen[0] = mgparm->grid[0]*((double) (mgparm->dime[0]-1));
01787         mgparm->glen[1] = mgparm->grid[1]*((double) (mgparm->dime[1]-1));
01788         mgparm->glen[2] = mgparm->grid[2]*((double) (mgparm->dime[2]-1));
01789     }

```

```

01790
01791 /* Check to see if he have any room left for this type of calculation, if
01792    so: set the calculation type, update the number of calculations of this type,
01793    and parse the rest of the section */
01794 if (thee->ncalc >= NOSH_MAXCALC) {
01795     Vnm_print(2, "Nosh: Too many calculations in this run!\n");
01796     Vnm_print(2, "Nosh: Current max is %d; ignoring this calculation\n",
01797               NOSH_MAXCALC);
01798     return 0;
01799 }
01800
01801 /* Get the next calculation object and increment the number of calculations */
01802 thee->calc[thee->ncalc] = NOsh_calc_ctor(NCT_MG);
01803 calc = thee->calc[thee->ncalc];
01804 (thee->ncalc)++;
01805
01806
01807
01808 /* Copy over contents of ELEC */
01809 NOsh_calc_copy(calc, elec);
01810
01811
01812 return 1;
01813 }
01814
01815 VPUBLIC int NOsh_setupCalcMGAUTO(
01816     NOsh *thee,
01817     NOsh_calc *elec
01818 ) {
01819
01820     NOsh_calc *calcf = VNULL;
01821     NOsh_calc *calcc = VNULL;
01822     double fgrid[3], cgrid[3];
01823     double d[3], minf[3], maxf[3], minc[3], maxc[3];
01824     double redfrac, redrat[3], td;
01825     int ifocus, nfocus, tnfocus[3];
01826     int j;
01827     int icalc;
01828     int dofex;
01829
01830     /* A comment about the coding style in this function. I use lots and lots
01831        and lots of pointer deferencing. I could (and probably should) save
01832        these in temporary variables. However, since there are so many Mgparm,
01833        etc. and NOsh_calc, etc. objects running around in this function, the
01834        current scheme is easiest to debug. */
01835
01836
01837     if (thee == VNULL) {
01838         Vnm_print(2, "NOsh_setupCalcMGAUTO: Got NULL thee!\n");
01839         return 0;
01840     }
01841     if (elec == VNULL) {
01842         Vnm_print(2, "NOsh_setupCalcMGAUTO: Got NULL elec!\n");
01843         return 0;
01844     }
01845     if (elec->mgparm == VNULL) {
01846         Vnm_print(2, "NOsh_setupCalcMGAUTO: Got NULL mgparm!\n");
01847         return 0;
01848     }
01849     if (elec->pbeparm == VNULL) {
01850         Vnm_print(2, "NOsh_setupCalcMGAUTO: Got NULL pbeparm!\n");
01851         return 0;
01852     }
01853
01854     Vnm_print(0, "NOsh_setupCalcMGAUTO(%s, %d): coarse grid center = %g %g %g\n",
01855               __FILE__, __LINE__,
01856               elec->mgparm->ccenter[0],
01857               elec->mgparm->ccenter[1],
01858               elec->mgparm->ccenter[2]);
01859     Vnm_print(0, "NOsh_setupCalcMGAUTO(%s, %d): fine grid center = %g %g %g\n",
01860               __FILE__, __LINE__,
01861               elec->mgparm->fcenter[0],
01862               elec->mgparm->fcenter[1],
01863               elec->mgparm->fcenter[2]);
01864
01865     /* Calculate the grid spacing on the coarse and fine levels */
01866     for (j=0; j<3; j++) {
01867         cgrid[j] = (elec->mgparm->cglen[j])/((double)(elec->mgparm->dime[j]-1));
01868         fgrid[j] = (elec->mgparm->fglen[j])/((double)(elec->mgparm->dime[j]-1));
01869         d[j] = elec->mgparm->fcenter[j] - elec->mgparm->ccenter[j];
01870     }

```

```

01871     Vnm_print(0, "Nosh_setupCalcMGAUTO (%s, %d): Coarse grid spacing = %g, %g, %g\n",
01872         __FILE__, __LINE__, cgrid[0], cgrid[1], cgrid[2]);
01873     Vnm_print(0, "Nosh_setupCalcMGAUTO (%s, %d): Fine grid spacing = %g, %g, %g\n",
01874         __FILE__, __LINE__, fgrid[0], fgrid[1], fgrid[2]);
01875     Vnm_print(0, "Nosh_setupCalcMGAUTO (%s, %d): Displacement between fine and \
01876 coarse grids = %g, %g, %g\n", __FILE__, __LINE__, d[0], d[1], d[2]);
01877
01878     /* Now calculate the number of focusing levels, never reducing the grid
01879 spacing by more than redfrac at each level */
01880     for (j=0; j<3; j++) {
01881         if (fgrid[j]/cgrid[j] < VREDFRAC) {
01882             redfrac = fgrid[j]/cgrid[j];
01883             td = log(redfrac)/log(VREDFRAC);
01884             tnfocus[j] = (int)ceil(td) + 1;
01885         } else tnfocus[j] = 2;
01886     }
01887     nfocus = VMAX2(VMAX2(tnfocus[0], tnfocus[1]), tnfocus[2]);
01888
01889     /* Now set redrat to the actual value by which the grid spacing is reduced
01890 at each level of focusing */
01891     for (j=0; j<3; j++) {
01892         redrat[j] = VPOW((fgrid[j]/cgrid[j]), 1.0/((double)nfocus-1.0));
01893     }
01894     Vnm_print(0, "Nosh: %d levels of focusing with %g, %g, %g reductions\n",
01895         nfocus, redrat[0], redrat[1], redrat[2]);
01896
01897     /* Now that we know how many focusing levels to use, we're ready to set up
01898 the parameter objects */
01899     if (nfocus > (NOSH_MAXCALC-(thee->ncalc))) {
01900         Vnm_print(2, "Nosh: Require more calculations than max (%d)!\n",
01901             NOSH_MAXCALC);
01902         return 0;
01903     }
01904
01905     for (ifocus=0; ifocus<nfocus; ifocus++) {
01906
01907         /* Generate the new calc object */
01908         icalc = thee->ncalc;
01909         thee->calc[icalc] = Nosh_calc_ctor(NCT_MG);
01910         (thee->ncalc)++;
01911
01912         /* This is the _current_ Nosh_calc object */
01913         calcf = thee->calc[icalc];
01914         /* This is the _previous_ Nosh_calc object */
01915         if (ifocus != 0) {
01916             calcc = thee->calc[icalc-1];
01917         } else {
01918             calcc = VNULL;
01919         }
01920
01921         /* Copy over most of the parameters from the ELEC object */
01922         Nosh_calc_copy(calcf, elec);
01923
01924         /* Set up the grid lengths and spacings */
01925         if (ifocus == 0) {
01926             for (j=0; j<3; j++) {
01927                 calcf->mgparm->grid[j] = cgrid[j];
01928                 calcf->mgparm->glen[j] = elec->mgparm->cglen[j];
01929             }
01930         } else {
01931             for (j=0; j<3; j++) {
01932                 calcf->mgparm->grid[j] = redrat[j]*(calcc->mgparm->grid[j]);
01933                 calcf->mgparm->glen[j] = redrat[j]*(calcc->mgparm->glen[j]);
01934             }
01935         }
01936         calcf->mgparm->setgrid = 1;
01937         calcf->mgparm->setglen = 1;
01938
01939         /* Get centers and centering method from coarse and fine meshes */
01940         if (ifocus == 0) {
01941             calcf->mgparm->cmeth = elec->mgparm->ccmeth;
01942             calcf->mgparm->centmol = elec->mgparm->ccentmol;
01943             for (j=0; j<3; j++) {
01944                 calcf->mgparm->center[j] = elec->mgparm->ccenter[j];
01945             }
01946         } else if (ifocus == (nfocus-1)) {
01947             calcf->mgparm->cmeth = elec->mgparm->fcmeth;
01948             calcf->mgparm->centmol = elec->mgparm->fcentmol;
01949             for (j=0; j<3; j++) {
01950                 calcf->mgparm->center[j] = elec->mgparm->fcenter[j];
01951             }
01952         }
01953     }

```

```

01952     } else {
01953         calcf->mgparm->cmeth = MCM_FOCUS;
01954         /* TEMPORARILY move the current grid center
01955            to the fine grid center. In general, this will move portions of
01956            the current mesh off the immediately-coarser mesh. We'll fix that
01957            in the next step. */
01958         for (j=0; j<3; j++) {
01959             calcf->mgparm->center[j] = elec->mgparm->fcenter[j];
01960         }
01961     }
01962
01963
01964     /* As mentioned above, it is highly likely that the previous "jump"
01965        to the fine grid center put portions of the current mesh off the
01966        previous (coarser) mesh. Fix this by displacing the current mesh
01967        back onto the previous coarser mesh. */
01968     if (ifocus != 0) {
01969         Vnm_print(0, "Nosh_setupCalcMGAUTO (%s, %d): starting mesh \
01970 repositioning.\n", __FILE__, __LINE__);
01971         Vnm_print(0, "Nosh_setupCalcMGAUTO (%s, %d): coarse mesh center = \
01972 %g %g %g\n", __FILE__, __LINE__,
01973                 calcc->mgparm->center[0],
01974                 calcc->mgparm->center[1],
01975                 calcc->mgparm->center[2]);
01976         Vnm_print(0, "Nosh_setupCalcMGAUTO (%s, %d): coarse mesh upper corner = \
01977 %g %g %g\n", __FILE__, __LINE__,
01978                 calcc->mgparm->center[0]+0.5*(calcc->mgparm->glen[0]),
01979                 calcc->mgparm->center[1]+0.5*(calcc->mgparm->glen[1]),
01980                 calcc->mgparm->center[2]+0.5*(calcc->mgparm->glen[2]));
01981         Vnm_print(0, "Nosh_setupCalcMGAUTO (%s, %d): coarse mesh lower corner = \
01982 %g %g %g\n", __FILE__, __LINE__,
01983                 calcc->mgparm->center[0]-0.5*(calcc->mgparm->glen[0]),
01984                 calcc->mgparm->center[1]-0.5*(calcc->mgparm->glen[1]),
01985                 calcc->mgparm->center[2]-0.5*(calcc->mgparm->glen[2]));
01986         Vnm_print(0, "Nosh_setupCalcMGAUTO (%s, %d): initial fine mesh upper corner = \
01987 %g %g %g\n", __FILE__, __LINE__,
01988                 calcf->mgparm->center[0]+0.5*(calcf->mgparm->glen[0]),
01989                 calcf->mgparm->center[1]+0.5*(calcf->mgparm->glen[1]),
01990                 calcf->mgparm->center[2]+0.5*(calcf->mgparm->glen[2]));
01991         Vnm_print(0, "Nosh_setupCalcMGAUTO (%s, %d): initial fine mesh lower corner = \
01992 %g %g %g\n", __FILE__, __LINE__,
01993                 calcf->mgparm->center[0]-0.5*(calcf->mgparm->glen[0]),
01994                 calcf->mgparm->center[1]-0.5*(calcf->mgparm->glen[1]),
01995                 calcf->mgparm->center[2]-0.5*(calcf->mgparm->glen[2]));
01996         for (j=0; j<3; j++) {
01997             /* Check if we've fallen off of the lower end of the mesh */
01998             dofix = 0;
01999             minf[j] = calcf->mgparm->center[j]
02000                 - 0.5*(calcf->mgparm->glen[j]);
02001             minc[j] = calcc->mgparm->center[j]
02002                 - 0.5*(calcc->mgparm->glen[j]);
02003             d[j] = minc[j] - minf[j];
02004             if (d[j] >= VSMALL) {
02005                 if (ifocus == (nfocus-1)) {
02006                     Vnm_print(2, "Nosh_setupCalcMGAUTO: Error! Finest \
02007 mesh has fallen off the coarser meshes!\n");
02008                     Vnm_print(2, "Nosh_setupCalcMGAUTO: difference in min %d-\
02009 direction = %g\n", j, d[j]);
02010                     Vnm_print(2, "Nosh_setupCalcMGAUTO: min fine = %g %g %g\n",
02011                             minf[0], minf[1], minf[2]);
02012                     Vnm_print(2, "Nosh_setupCalcMGAUTO: min coarse = %g %g %g\n",
02013                             minc[0], minc[1], minc[2]);
02014                     VASSERT(0);
02015                 } else {
02016                     Vnm_print(0, "Nosh_setupCalcMGAUTO (%s, %d): ifocus = %d, \
02017 fixing mesh min violation (%g in %d-direction).\n", __FILE__, __LINE__, ifocus,
02018                             d[j], j);
02019                     calcf->mgparm->center[j] += d[j];
02020                     dofix = 1;
02021                 }
02022             }
02023             /* Check if we've fallen off of the upper end of the mesh */
02024             maxf[j] = calcf->mgparm->center[j] \
02025                 + 0.5*(calcf->mgparm->glen[j]);
02026             maxc[j] = calcc->mgparm->center[j] \
02027                 + 0.5*(calcc->mgparm->glen[j]);
02028             d[j] = maxf[j] - maxc[j];
02029             if (d[j] >= VSMALL) {
02030                 if (ifocus == (nfocus-1)) {
02031                     Vnm_print(2, "Nosh_setupCalcMGAUTO: Error! Finest \
02032 mesh has fallen off the coarser meshes!\n");

```

```

02033         Vnm_print(2, "Nosh_setupCalcMGAUTO:  difference in %d-\
02034 direction = %g\n", j, d[j]);
02035         VASSERT(0);
02036     } else {
02037         /* If we already fixed the lower boundary and we now need
02038         to fix the upper boundary, we have a serious problem. */
02039         if (dofix) {
02040             Vnm_print(2, "Nosh_setupCalcMGAUTO:  Error!  Both \
02041 ends of the finer mesh do not fit in the bigger mesh!\n");
02042             VASSERT(0);
02043         }
02044         Vnm_print(0, "Nosh_setupCalcMGAUTO(%s, %d):  ifocus = %d, \
02045 fixing mesh max violation (%g in %d-direction).\n", __FILE__, __LINE__, ifocus,
02046             d[j], j);
02047         calcf->mgparm->center[j] -= d[j];
02048         dofix = 1;
02049     }
02050 }
02051 }
02052 Vnm_print(0, "Nosh_setupCalcMGAUTO (%s, %d):  final fine mesh upper corner = \
02053 %g %g %g\n", __FILE__, __LINE__,
02054     calcf->mgparm->center[0]+0.5*(calcf->mgparm->glen[0]),
02055     calcf->mgparm->center[1]+0.5*(calcf->mgparm->glen[1]),
02056     calcf->mgparm->center[2]+0.5*(calcf->mgparm->glen[2]));
02057 Vnm_print(0, "Nosh_setupCalcMGAUTO (%s, %d):  final fine mesh lower corner = \
02058 %g %g %g\n", __FILE__, __LINE__,
02059     calcf->mgparm->center[0]-0.5*(calcf->mgparm->glen[0]),
02060     calcf->mgparm->center[1]-0.5*(calcf->mgparm->glen[1]),
02061     calcf->mgparm->center[2]-0.5*(calcf->mgparm->glen[2]));
02062 }
02063
02064 /* Finer levels have focusing boundary conditions */
02065 if (ifocus != 0) calcf->pbeparm->bcfl = BCFL_FOCUS;
02066
02067 /* Only the finest level handles I/O and needs to worry about disjoint
02068 partitioning */
02069 if (ifocus != (nfocus-1)) calcf->pbeparm->numwrite = 0;
02070
02071 /* Reset boundary flags for everything except parallel focusing */
02072 if (calcf->mgparm->type != MCT_PARALLEL) {
02073     Vnm_print(0, "Nosh_setupMGAUTO:  Resetting boundary flags\n");
02074     for (j=0; j<6; j++) calcf->mgparm->partDisjOwnSide[j] = 0;
02075     for (j=0; j<3; j++) {
02076         calcf->mgparm->partDisjCenter[j] = 0;
02077         calcf->mgparm->partDisjLength[j] = calcf->mgparm->glen[j];
02078     }
02079 }
02080
02081 calcf->mgparm->parsed = 1;
02082 }
02083
02084 return 1;
02085 }
02086
02087 }
02088
02089 /* Author:  Nathan Baker and Todd Dolinsky */
02090 VPUBLIC int Nosh_setupCalcMGPARA(
02091     NOsh *thee,
02092     NOsh_calc *elec
02093 ) {
02094
02095     /* NEW (25-Jul-2006):  This code should produce modify the ELEC statement
02096     and pass it on to MGAUTO for further processing. */
02097
02098     MGparm *mgparm = VNULL;
02099     double ofrac;
02100     double hx, hy, hzed;
02101     double xofrac, yofrac, zofrac;
02102     int rank, size, npx, npy, npz, nproc, ip, jp, kp;
02103     int xeffGlob, yeffGlob, zeffGlob, xDisj, yDisj, zDisj;
02104     int xigminDisj, xigmaxDisj, yigminDisj, yigmaxDisj, zigminDisj, zigmaxDisj;
02105     int xigminOlap, xigmaxOlap, yigminOlap, yigmaxOlap, zigminOlap, zigmaxOlap;
02106     int xOlapReg, yOlapReg, zOlapReg;
02107     double xlenDisj, ylenDisj, zlenDisj;
02108     double xcentDisj, ycentDisj, zcentDisj;
02109     double xcentOlap, ycentOlap, zcentOlap;
02110     double xlenOlap, ylenOlap, zlenOlap;
02111     double xminOlap, xmaxOlap, yminOlap, ymaxOlap, zminOlap, zmaxOlap;
02112     double xminDisj, xmaxDisj, yminDisj, ymaxDisj, zminDisj, zmaxDisj;
02113     double xcent, ycent, zcent;

```



```

02114
02115     /* Grab some useful variables */
02116     VASSERT(thee != VNULL);
02117     VASSERT(elec != VNULL);
02118     mgparm = elec->mgparm;
02119     VASSERT(mgparm != VNULL);
02120
02121     /* Grab some useful variables */
02122     ofrac = mgparm->ofrac;
02123     npx = mgparm->pdime[0];
02124     npy = mgparm->pdime[1];
02125     npz = mgparm->pdime[2];
02126     nproc = npx*npy*npz;
02127
02128     /* If this is not an asynchronous calculation, then we need to make sure we
02129        have all the necessary MPI information */
02130     if (mgparm->setasync == 0) {
02131
02132 #ifndef HAVE_MPI_H
02133
02134         Vnm_tprint(2, "Nosh_setupCalcMGPARA: Oops! You're trying to perform \
02135 an 'mg-para' (parallel) calculation\n");
02136         Vnm_tprint(2, "Nosh_setupCalcMGPARA: with a version of APBS that wasn't \
02137 compiled with MPI!\n");
02138         Vnm_tprint(2, "Nosh_setupCalcMGPARA: Perhaps you meant to use the \
02139 'async' flag?\n");
02140         Vnm_tprint(2, "Nosh_setupCalcMGPARA: Bailing out!\n");
02141
02142         return 0;
02143
02144 #endif
02145
02146         rank = thee->proc_rank;
02147         size = thee->proc_size;
02148         Vnm_print(0, "Nosh_setupCalcMGPARA: Hello from processor %d of %d\n", rank,
02149                 size);
02150
02151         /* Check to see if we have too many processors. If so, then simply set
02152            this processor to duplicating the work of processor 0. */
02153         if (rank > (nproc-1)) {
02154             Vnm_print(2, "Nosh_setupMGPARA: There are more processors available than\
02155 the %d you requested.\n", nproc);
02156             Vnm_print(2, "Nosh_setupMGPARA: Eliminating processor %d\n", rank);
02157             thee->bogus = 1;
02158             rank = 0;
02159         }
02160
02161         /* Check to see if we have too few processors. If so, this is a fatal
02162            error. */
02163         if (size < nproc) {
02164             Vnm_print(2, "Nosh_setupMGPARA: There are too few processors (%d) to \
02165 satisfy requirements (%d)\n", size, nproc);
02166             return 0;
02167         }
02168
02169         Vnm_print(0, "Nosh_setupMGPARA: Hello (again) from processor %d of %d\n",
02170                 rank, size);
02171
02172     } else { /* Setting up for an asynchronous calculation. */
02173
02174         rank = mgparm->async;
02175
02176         thee->ispara = 1;
02177         thee->proc_rank = rank;
02178
02179         /* Check to see if the async id is greater than the number of
02180            * processors. If so, this is a fatal error. */
02181         if (rank > (nproc-1)) {
02182             Vnm_print(2, "Nosh_setupMGPARA: The processor id you requested (%d) \
02183 is not within the range of processors available (0-%d)\n", rank, (nproc-1));
02184             return 0;
02185         }
02186     }
02187
02188     /* Calculate the processor's coordinates in the processor grid */
02189     kp = (int) floor(rank / (npx*npy));
02190     jp = (int) floor((rank - kp*npx*npy) / npx);
02191     ip = rank - kp*npx*npy - jp*npx;
02192     Vnm_print(0, "Nosh_setupMGPARA: Hello world from PE (%d, %d, %d)\n",
02193             ip, jp, kp);
02194

```

```

02195      /* Calculate effective overlap fractions for uneven processor distributions */
02196      if (npx == 1) xofrac = 0.0;
02197      else xofrac = ofrac;
02198      if (npz == 1) yofrac = 0.0;
02199      else yofrac = ofrac;
02200      if (npz == 1) zofrac = 0.0;
02201      else zofrac = ofrac;
02202
02203      /* Calculate the global grid size and spacing */
02204      xDisj = (int)VFFLOOR(mgparm->dime[0]/(1 + 2*xofrac) + 0.5);
02205      xeffGlob = npx*xDisj;
02206      hx = mgparm->fglen[0]/(double)(xeffGlob-1);
02207      yDisj = (int)VFFLOOR(mgparm->dime[1]/(1 + 2*yofrac) + 0.5);
02208      yeffGlob = npy*yDisj;
02209      hy = mgparm->fglen[1]/(double)(yeffGlob-1);
02210      zDisj = (int)VFFLOOR(mgparm->dime[2]/(1 + 2*zofrac) + 0.5);
02211      zeffGlob = npz*zDisj;
02212      hzed = mgparm->fglen[2]/(double)(zeffGlob-1);
02213      Vnm_print(0, "Nosh_setupMGPARA: Global Grid size = (%d, %d, %d)\n",
02214                xeffGlob, yeffGlob, zeffGlob);
02215      Vnm_print(0, "Nosh_setupMGPARA: Global Grid Spacing = (%.3f, %.3f, %.3f)\n",
02216                hx, hy, hzed);
02217      Vnm_print(0, "Nosh_setupMGPARA: Processor Grid Size = (%d, %d, %d)\n",
02218                xDisj, yDisj, zDisj);
02219
02220      /* Calculate the maximum and minimum processor grid points */
02221      xigminDisj = ip*xDisj;
02222      xigmaxDisj = xigminDisj + xDisj - 1;
02223      yigminDisj = jp*yDisj;
02224      yigmaxDisj = yigminDisj + yDisj - 1;
02225      zigminDisj = kp*zDisj;
02226      zigmaxDisj = zigminDisj + zDisj - 1;
02227      Vnm_print(0, "Nosh_setupMGPARA: Min Grid Points for this proc. (%d, %d, %d)\n",
02228                xigminDisj, yigminDisj, zigminDisj);
02229      Vnm_print(0, "Nosh_setupMGPARA: Max Grid Points for this proc. (%d, %d, %d)\n",
02230                xigmaxDisj, yigmaxDisj, zigmaxDisj);
02231
02232      /* Calculate the disjoint partition length and center displacement */
02233      xminDisj = VMAX2(hx*(xigminDisj-0.5), 0.0);
02234      xmaxDisj = VMIN2(hx*(xigmaxDisj+0.5), mgparm->fglen[0]);
02235      xlenDisj = xmaxDisj - xminDisj;
02236      yminDisj = VMAX2(hy*(yigminDisj-0.5), 0.0);
02237      ymaxDisj = VMIN2(hy*(yigmaxDisj+0.5), mgparm->fglen[1]);
02238      ylenDisj = ymaxDisj - yminDisj;
02239      zminDisj = VMAX2(hzed*(zigminDisj-0.5), 0.0);
02240      zmaxDisj = VMIN2(hzed*(zigmaxDisj+0.5), mgparm->fglen[2]);
02241      zlenDisj = zmaxDisj - zminDisj;
02242
02243      xcent = 0.5*mgparm->fglen[0];
02244      ycent = 0.5*mgparm->fglen[1];
02245      zcent = 0.5*mgparm->fglen[2];
02246
02247      xcentDisj = xminDisj + 0.5*xlenDisj - xcent;
02248      ycentDisj = yminDisj + 0.5*ylenDisj - ycent;
02249      zcentDisj = zminDisj + 0.5*zlenDisj - zcent;
02250      if (VABS(xcentDisj) < VSMALL) xcentDisj = 0.0;
02251      if (VABS(ycentDisj) < VSMALL) ycentDisj = 0.0;
02252      if (VABS(zcentDisj) < VSMALL) zcentDisj = 0.0;
02253
02254      Vnm_print(0, "Nosh_setupMGPARA: Disj part length = (%g, %g, %g)\n",
02255                xlenDisj, ylenDisj, zlenDisj);
02256      Vnm_print(0, "Nosh_setupMGPARA: Disj part center displacement = (%g, %g, %g)\n",
02257                xcentDisj, ycentDisj, zcentDisj);
02258
02259      /* Calculate the overlapping partition length and center displacement */
02260      xOlapReg = 0;
02261      yOlapReg = 0;
02262      zOlapReg = 0;
02263      if (npx != 1) xOlapReg = (int)VFFLOOR(xofrac*mgparm->fglen[0]/npx/hx + 0.5) + 1;
02264      if (npy != 1) yOlapReg = (int)VFFLOOR(yofrac*mgparm->fglen[1]/npy/hy + 0.5) + 1;
02265      if (npz != 1) zOlapReg = (int)VFFLOOR(zofrac*mgparm->fglen[2]/npz/hzed + 0.5) + 1;
02266
02267      Vnm_print(0, "Nosh_setupMGPARA: No. of Grid Points in Overlap (%d, %d, %d)\n",
02268                xOlapReg, yOlapReg, zOlapReg);
02269
02270      if (ip == 0) xigminOlap = 0;
02271      else if (ip == (npx - 1)) xigminOlap = xeffGlob - mgparm->dime[0];
02272      else xigminOlap = xigminDisj - xOlapReg;
02273      xigmaxOlap = xigminOlap + mgparm->dime[0] - 1;
02274
02275

```

```

02276     if (jp == 0) yigminOlap = 0;
02277     else if (jp == (npz - 1)) yigminOlap = yeffGlob - mgparm->dime[1];
02278     else yigminOlap = yigminDisj - yOlapReg;
02279     yigmaxOlap = yigminOlap + mgparm->dime[1] - 1;
02280
02281     if (kp == 0) zigminOlap = 0;
02282     else if (kp == (npz - 1)) zigminOlap = zeffGlob - mgparm->dime[2];
02283     else zigminOlap = zigminDisj - zOlapReg;
02284     zigmaxOlap = zigminOlap + mgparm->dime[2] - 1;
02285
02286     Vnm_print(0, "Nosh_setupMGPARA: Min Grid Points with Overlap (%d, %d, %d)\n",
02287               xigminOlap, yigminOlap, zigminOlap);
02288     Vnm_print(0, "Nosh_setupMGPARA: Max Grid Points with Overlap (%d, %d, %d)\n",
02289               xigmaxOlap, yigmaxOlap, zigmaxOlap);
02290
02291     xminOlap = hx * xigminOlap;
02292     xmaxOlap = hx * xigmaxOlap;
02293     yminOlap = hy * yigminOlap;
02294     ymaxOlap = hy * yigmaxOlap;
02295     zminOlap = hzed * zigminOlap;
02296     zmaxOlap = hzed * zigmaxOlap;
02297
02298     xlenOlap = xmaxOlap - xminOlap;
02299     ylenOlap = ymaxOlap - yminOlap;
02300     zlenOlap = zmaxOlap - zminOlap;
02301
02302     xcentOlap = (xminOlap + 0.5*xlenOlap) - xcent;
02303     ycentOlap = (yminOlap + 0.5*ylenOlap) - ycent;
02304     zcentOlap = (zminOlap + 0.5*zlenOlap) - zcent;
02305     if (VABS(xcentOlap) < VSMALL) xcentOlap = 0.0;
02306     if (VABS(ycentOlap) < VSMALL) ycentOlap = 0.0;
02307     if (VABS(zcentOlap) < VSMALL) zcentOlap = 0.0;
02308
02309     Vnm_print(0, "Nosh_setupMGPARA: Olap part length = (%g, %g, %g)\n",
02310               xlenOlap, ylenOlap, zlenOlap);
02311     Vnm_print(0, "Nosh_setupMGPARA: Olap part center displacement = (%g, %g, %g)\n",
02312               xcentOlap, ycentOlap, zcentOlap);
02313
02314
02315     /* Calculate the boundary flags:
02316        Flags are set to 1 when another processor is present along the boundary
02317        Flags are otherwise set to 0. */
02318
02319     if (ip == 0) mgparm->partDisjOwnSide[VAPBS_LEFT] = 0;
02320     else mgparm->partDisjOwnSide[VAPBS_LEFT] = 1;
02321     if (ip == (npz-1)) mgparm->partDisjOwnSide[VAPBS_RIGHT] = 0;
02322     else mgparm->partDisjOwnSide[VAPBS_RIGHT] = 1;
02323     if (jp == 0) mgparm->partDisjOwnSide[VAPBS_BACK] = 0;
02324     else mgparm->partDisjOwnSide[VAPBS_BACK] = 1;
02325     if (jp == (npz-1)) mgparm->partDisjOwnSide[VAPBS_FRONT] = 0;
02326     else mgparm->partDisjOwnSide[VAPBS_FRONT] = 1;
02327     if (kp == 0) mgparm->partDisjOwnSide[VAPBS_DOWN] = 0;
02328     else mgparm->partDisjOwnSide[VAPBS_DOWN] = 1;
02329     if (kp == (npz-1)) mgparm->partDisjOwnSide[VAPBS_UP] = 0;
02330     else mgparm->partDisjOwnSide[VAPBS_UP] = 1;
02331
02332     Vnm_print(0, "Nosh_setupMGPARA: partDisjOwnSide[LEFT] = %d\n",
02333               mgparm->partDisjOwnSide[VAPBS_LEFT]);
02334     Vnm_print(0, "Nosh_setupMGPARA: partDisjOwnSide[RIGHT] = %d\n",
02335               mgparm->partDisjOwnSide[VAPBS_RIGHT]);
02336     Vnm_print(0, "Nosh_setupMGPARA: partDisjOwnSide[FRONT] = %d\n",
02337               mgparm->partDisjOwnSide[VAPBS_FRONT]);
02338     Vnm_print(0, "Nosh_setupMGPARA: partDisjOwnSide[BACK] = %d\n",
02339               mgparm->partDisjOwnSide[VAPBS_BACK]);
02340     Vnm_print(0, "Nosh_setupMGPARA: partDisjOwnSide[UP] = %d\n",
02341               mgparm->partDisjOwnSide[VAPBS_UP]);
02342     Vnm_print(0, "Nosh_setupMGPARA: partDisjOwnSide[DOWN] = %d\n",
02343               mgparm->partDisjOwnSide[VAPBS_DOWN]);
02344
02345     /* Set the mesh parameters */
02346     mgparm->fglen[0] = xlenOlap;
02347     mgparm->fglen[1] = ylenOlap;
02348     mgparm->fglen[2] = zlenOlap;
02349     mgparm->partDisjLength[0] = xlenDisj;
02350     mgparm->partDisjLength[1] = ylenDisj;
02351     mgparm->partDisjLength[2] = zlenDisj;
02352     mgparm->partDisjCenter[0] = mgparm->fcenter[0] + xcentDisj;
02353     mgparm->partDisjCenter[1] = mgparm->fcenter[1] + ycentDisj;
02354     mgparm->partDisjCenter[2] = mgparm->fcenter[2] + zcentDisj;
02355     mgparm->fcenter[0] += xcentOlap;
02356     mgparm->fcenter[1] += ycentOlap;

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```

02357     mgparm->fcenter[2] += zcentOlap;
02358
02359     Vnm_print(0, "Nosh_setupCalcMGPARA (%s, %d): Set up *relative* partition \
02360 centers...\n", __FILE__, __LINE__);
02361     Vnm_print(0, "Nosh_setupCalcMGPARA (%s, %d): Absolute centers will be set \
02362 in Nosh_setupMGAUTO\n", __FILE__, __LINE__);
02363     Vnm_print(0, "Nosh_setupCalcMGPARA (%s, %d): partDisjCenter = %g %g %g\n",
02364             __FILE__, __LINE__,
02365             mgparm->partDisjCenter[0],
02366             mgparm->partDisjCenter[1],
02367             mgparm->partDisjCenter[2]);
02368     Vnm_print(0, "Nosh_setupCalcMGPARA (%s, %d): ccenter = %g %g %g\n",
02369             __FILE__, __LINE__,
02370             mgparm->ccenter[0],
02371             mgparm->ccenter[1],
02372             mgparm->ccenter[2]);
02373     Vnm_print(0, "Nosh_setupCalcMGPARA (%s, %d): fcenter = %g %g %g\n",
02374             __FILE__, __LINE__,
02375             mgparm->fcenter[0],
02376             mgparm->fcenter[1],
02377             mgparm->fcenter[2]);
02378
02379
02380     /* Setup the automatic focusing calculations associated with this processor */
02381     return Nosh_setupCalcMGAUTO(thee, elec);
02382
02383 }
02384
02385 VPUBLIC int Nosh_parseFEM(
02386     Nosh *thee,
02387     Vio *sock,
02388     Nosh_calc *elec
02389 ) {
02390
02391     char tok[VMAX_BUF_SIZE];
02392     FEMparm *feparm = VNULL;
02393     PBEParm *pbeparm = VNULL;
02394     int rc;
02395     Vrc_Codes vrc;
02396
02397     /* Check the arguments */
02398     if (thee == VNULL) {
02399         Vnm_print(2, "Nosh_parseFEM: Got NULL thee!\n");
02400         return 0;
02401     }
02402     if (sock == VNULL) {
02403         Vnm_print(2, "Nosh_parseFEM: Got pointer to NULL socket!\n");
02404         return 0;
02405     }
02406     if (elec == VNULL) {
02407         Vnm_print(2, "Nosh_parseFEM: Got pointer to NULL elec object!\n");
02408         return 0;
02409     }
02410     feparm = elec->feparm;
02411     if (feparm == VNULL) {
02412         Vnm_print(2, "Nosh_parseFEM: Got pointer to NULL feparm object!\n");
02413         return 0;
02414     }
02415     pbeparm = elec->pbeparm;
02416     if (pbeparm == VNULL) {
02417         Vnm_print(2, "Nosh_parseFEM: Got pointer to NULL pbeparm object!\n");
02418         return 0;
02419     }
02420
02421     Vnm_print(0, "Nosh_parseFEM: Parsing parameters for FEM calculation\n");
02422
02423     /* Start snarfing tokens from the input stream */
02424     rc = 1;
02425     while (Vio_scanf(sock, "%s", tok) == 1) {
02426
02427         Vnm_print(0, "Nosh_parseFEM: Parsing %s...\n", tok);
02428
02429         /* See if it's an END token */
02430         if (Vstring_strcasecmp(tok, "end") == 0) {
02431             feparm->parsed = 1;
02432             pbeparm->parsed = 1;
02433             rc = 1;
02434             break;
02435         }
02436
02437         /* Pass the token through a series of parsers */

```

```

02438     rc = PBEParm_parseToken(pbeparm, tok, sock);
02439     if (rc == -1) {
02440         Vnm_print(0, "Nosh_parseFEM: parsePBE error!\n");
02441         break;
02442     } else if (rc == 0) {
02443         /* Pass the token to the generic MG parser */
02444         vrc = FEMparm_parseToken(feparm, tok, sock);
02445         if (vrc == VRC_FAILURE) {
02446             Vnm_print(0, "Nosh_parseFEM: parseMG error!\n");
02447             break;
02448         } else if (vrc == VRC_WARNING) {
02449             /* We ran out of parsers! */
02450             Vnm_print(2, "Nosh: Unrecognized keyword: %s\n", tok);
02451             break;
02452         }
02453     }
02454 }
02455
02456 /* Handle various errors arising in the token-snarfing loop -- these all
02457  * just result in simple returns right now */
02458 if (rc == -1) return 0;
02459 if (rc == 0) return 0;
02460
02461 /* Check the status of the parameter objects */
02462 if ((!FEMparm_check(feparm)) || (!PBEParm_check(pbeparm))) {
02463     Vnm_print(2, "Nosh: FEM parameters not set correctly!\n");
02464     return 0;
02465 }
02466
02467 return 1;
02468 }
02469 }
02470
02471 VPRIVATE int Nosh_setupCalcFEMANUAL(
02472     Nosh *thee,
02473     Nosh_calc *elec
02474 ) {
02475
02476     FEMparm *feparm = VNULL;
02477     PBEParm *pbeparm = VNULL;
02478     Nosh_calc *calc = VNULL;
02479
02480     VASSERT(thee != VNULL);
02481     VASSERT(elec != VNULL);
02482     feparm = elec->feparm;
02483     VASSERT(feparm != VNULL);
02484     pbeparm = elec->pbeparm;
02485     VASSERT(pbeparm);
02486
02487     /* Check to see if he have any room left for this type of
02488      * calculation, if so: set the calculation type, update the number
02489      * of calculations of this type, and parse the rest of the section
02490      */
02491     if (thee->ncalc >= NOSH_MAXCALC) {
02492         Vnm_print(2, "Nosh: Too many calculations in this run!\n");
02493         Vnm_print(2, "Nosh: Current max is %d; ignoring this calculation\n",
02494             NOSH_MAXCALC);
02495         return 0;
02496     }
02497     thee->calc[thee->ncalc] = Nosh_calc_ctor(NCT_FEM);
02498     calc = thee->calc[thee->ncalc];
02499     (thee->ncalc)++;
02500
02501     /* Copy over contents of ELEC */
02502     Nosh_calc_copy(calc, elec);
02503
02504
02505     return 1;
02506 }
02507
02508 VPUBLIC int Nosh_parseAPOL(
02509     Nosh *thee,
02510     Vio *sock,
02511     Nosh_calc *elec
02512 ) {
02513
02514     char tok[VMAX_BUFSIZE];
02515     APOLparm *apolparm = VNULL;
02516     int rc;
02517
02518     /* Check the arguments */

```

```

02519     if (thee == VNULL) {
02520         Vnm_print(2, "Nosh_parseAPOL: Got NULL thee!\n");
02521         return 0;
02522     }
02523     if (sock == VNULL) {
02524         Vnm_print(2, "Nosh_parseAPOL: Got pointer to NULL socket!\n");
02525         return 0;
02526     }
02527     if (elec == VNULL) {
02528         Vnm_print(2, "Nosh_parseAPOL: Got pointer to NULL elec object!\n");
02529         return 0;
02530     }
02531     apolparm = elec->apolparm;
02532     if (apolparm == VNULL) {
02533         Vnm_print(2, "Nosh_parseAPOL: Got pointer to NULL apolparm object!\n");
02534         return 0;
02535     }
02536
02537     Vnm_print(0, "Nosh_parseAPOL: Parsing parameters for APOL calculation\n");
02538
02539     /* Start snarfing tokens from the input stream */
02540     rc = 1;
02541     while (Vio_scanf(sock, "%s", tok) == 1) {
02542
02543         Vnm_print(0, "Nosh_parseAPOL: Parsing %s...\n", tok);
02544         /* See if it's an END token */
02545         if (Vstring_strcasecmp(tok, "end") == 0) {
02546             apolparm->parsed = 1;
02547             rc = 1;
02548             break;
02549         }
02550
02551         /* Pass the token through a series of parsers */
02552         /* Pass the token to the generic non-polar parser */
02553         rc = APOLparm_parseToken(apolparm, tok, sock);
02554         if (rc == -1) {
02555             Vnm_print(0, "Nosh_parseFEM: parseMG error!\n");
02556             break;
02557         } else if (rc == 0) {
02558             /* We ran out of parsers! */
02559             Vnm_print(2, "Nosh: Unrecognized keyword: %s\n", tok);
02560             break;
02561         }
02562     }
02563
02564     /* Handle various errors arising in the token-snarfing loop -- these all
02565      * just result in simple returns right now */
02566     if (rc == -1) return 0;
02567     if (rc == 0) return 0;
02568
02569     /* Check the status of the parameter objects */
02570     if (!APOLparm_check(apolparm)) {
02571         Vnm_print(2, "Nosh: APOL parameters not set correctly!\n");
02572         return 0;
02573     }
02574
02575     return 1;
02576 }
02577
02578 }
02579
02580
02581 VPRIVATE int Nosh_setupCalcAPOL(
02582     Nosh *thee,
02583     Nosh_calc *apol
02584 ) {
02585
02586     Nosh_calc *calc = VNULL;
02587
02588     VASSERT(thee != VNULL);
02589     VASSERT(apol != VNULL);
02590
02591     /* Check to see if he have any room left for this type of
02592      * calculation, if so: set the calculation type, update the number
02593      * of calculations of this type, and parse the rest of the section
02594      */
02595     if (thee->ncalc >= NOSH_MAXCALC) {
02596         Vnm_print(2, "Nosh: Too many calculations in this run!\n");
02597         Vnm_print(2, "Nosh: Current max is %d; ignoring this calculation\n",
02598                 NOSH_MAXCALC);
02599         return 0;

```

```

02600     }
02601     thee->calc[thee->ncalc] = NOsh_calc_ctor(NCT_APOL);
02602     calc = thee->calc[thee->ncalc];
02603     (thee->ncalc)++;
02604
02605     /* Copy over contents of APOL */
02606     NOsh_calc_copy(calc, apol);
02607
02608     return 1;
02609 }
02610
02611
02612 VPRIVATE int NOsh_setupCalcBEMMANUAL(
02613     NOsh *thee,
02614     NOsh_calc *elec
02615 ) {
02616
02617     BEMparm *bemparm = VNULL;
02618     PBEParm *pbeparm = VNULL;
02619     NOsh_calc *calc = VNULL;
02620
02621     if (thee == VNULL) {
02622         Vnm_print(2, "NOsh_setupCalcBEMMANUAL: Got NULL thee!\n");
02623         return 0;
02624     }
02625     if (elec == VNULL) {
02626         Vnm_print(2, "NOsh_setupCalcBEMMANUAL: Got NULL calc!\n");
02627         return 0;
02628     }
02629     bemparm = elec->bemparm;
02630     if (bemparm == VNULL) {
02631         Vnm_print(2, "NOsh_setupCalcBEMMANUAL: Got NULL bemparm -- was this calculation \
02632 set up?\n");
02633         return 0;
02634     }
02635     pbeparm = elec->pbeparm;
02636     if (pbeparm == VNULL) {
02637         Vnm_print(2, "NOsh_setupCalcBEMMANUAL: Got NULL pbeparm -- was this calculation \
02638 set up?\n");
02639         return 0;
02640     }
02641
02642     /* Set up missing BEM parameters */
02643     if (bemparm->settree_order == 0) {
02644         bemparm->tree_order=1;
02645     }
02646
02647     if (bemparm->settree_n0 == 0) {
02648         bemparm->tree_n0=500;
02649     }
02650
02651     if (bemparm->setmac == 0) {
02652         bemparm->mac=0.8;
02653     }
02654
02655     /* Check to see if he have any room left for this type of calculation, if
02656 so: set the calculation type, update the number of calculations of this type,
02657 and parse the rest of the section */
02658     if (thee->ncalc >= NOSH_MAXCALC) {
02659         Vnm_print(2, "NOsh: Too many calculations in this run!\n");
02660         Vnm_print(2, "NOsh: Current max is %d; ignoring this calculation\n",
02661             NOSH_MAXCALC);
02662         return 0;
02663     }
02664
02665     /* Get the next calculation object and increment the number of calculations */
02666     thee->calc[thee->ncalc] = NOsh_calc_ctor(NCT_BEM);
02667     calc = thee->calc[thee->ncalc];
02668     (thee->ncalc)++;
02669
02670     /* Copy over contents of ELEC */
02671     NOsh_calc_copy(calc, elec);
02672
02673     return 1;
02674 }
02675
02676
02677 VPRIVATE int NOsh_setupCalcGEOFLOWMANUAL(
02678     NOsh *thee,
02679     NOsh_calc *elec
02680 ) {

```

```

02681
02682     GEOFLOWparm *parm = VNULL;
02683     APOLparm *apolparm = VNULL;
02684     PBEParm *pbeparm = VNULL;
02685     Nosh_calc *calc = VNULL;
02686
02687     if (thee == VNULL) {
02688         Vnm_print(2, "Nosh_setupCalcGEOFLOWMANUAL: Got NULL thee!\n");
02689         return 0;
02690     }
02691     if (elec == VNULL) {
02692         Vnm_print(2, "Nosh_setupCalcGEOFLOWMANUAL: Got NULL calc!\n");
02693         return 0;
02694     }
02695     parm = elec->geoflowparm;
02696     if (parm == VNULL) {
02697         Vnm_print(2, "Nosh_setupCalcGEOFLOWMANUAL: Got NULL geoflowparm -- was this calculation \
02698 set up?\n");
02699         return 0;
02700     }
02701     apolparm = elec->apolparm;
02702     if (parm == VNULL) {
02703         Vnm_print(2, "Nosh_setupCalcGEOFLOWMANUAL: Got NULL apolparm -- was this calculation \
02704 set up?\n");
02705         return 0;
02706     }
02707     pbeparm = elec->pbeparm;
02708     if (pbeparm == VNULL) {
02709         Vnm_print(2, "Nosh_setupCalcGEOFLOWMANUAL: Got NULL pbeparm -- was this calculation \
02710 set up?\n");
02711         return 0;
02712     }
02713
02714     /* Check to see if he have any room left for this type of calculation, if
02715        so: set the calculation type, update the number of calculations of this type,
02716        and parse the rest of the section */
02717     if (thee->ncalc >= NOSH_MAXCALC) {
02718         Vnm_print(2, "Nosh: Too many calculations in this run!\n");
02719         Vnm_print(2, "Nosh: Current max is %d; ignoring this calculation\n",
02720                 NOSH_MAXCALC);
02721         return 0;
02722     }
02723
02724     /* Get the next calculation object and increment the number of calculations */
02725     thee->calc[thee->ncalc] = Nosh_calc_ctor(NCT_GEOFLOW);
02726     calc = thee->calc[thee->ncalc];
02727     (thee->ncalc)++;
02728
02729     /* Copy over contents of ELEC */
02730     Nosh_calc_copy(calc, elec);
02731
02732     return 1;
02733 }
02734
02735 VPRIVATE int Nosh_setupCalcPBAMAUTO(
02736     Nosh *thee,
02737     Nosh_calc *elec
02738 ) {
02739
02740     PBAMparm *parm = VNULL;
02741     PBEParm *pbeparm = VNULL;
02742     Nosh_calc *calc = VNULL;
02743
02744     if (thee == VNULL) {
02745         Vnm_print(2, "Nosh_setupCalcPBAMAUTO: Got NULL thee!\n");
02746         return 0;
02747     }
02748     if (elec == VNULL) {
02749         Vnm_print(2, "Nosh_setupCalcPBAMAUTO: Got NULL calc!\n");
02750         return 0;
02751     }
02752     parm = elec->pbamparm;
02753     if (parm == VNULL) {
02754         Vnm_print(2, "Nosh_setupCalcPBAMAUTO: Got NULL pbamparm -- was this calculation \
02755 set up?\n");
02756         return 0;
02757     }
02758     pbeparm = elec->pbeparm;
02759     if (pbeparm == VNULL) {
02760         Vnm_print(2, "Nosh_setupCalcPBAMAUTO: Got NULL pbeparm -- was this calculation \
02761 set up?\n");

```



```

02762     return 0;
02763 }
02764
02765 /* Check to see if he have any room left for this type of calculation, if
02766    so: set the calculation type, update the number of calculations of this type,
02767    and parse the rest of the section */
02768 if (thee->ncalc >= NOSH_MAXCALC) {
02769     Vnm_print(2, "Nosh: Too many calculations in this run!\n");
02770     Vnm_print(2, "Nosh: Current max is %d; ignoring this calculation\n",
02771             NOSH_MAXCALC);
02772     return 0;
02773 }
02774
02775 /* Get the next calculation object and increment the number of calculations */
02776 thee->calc[thee->ncalc] = Nosh_calc_ctor(NCT_PBAM);
02777 calc = thee->calc[thee->ncalc];
02778 (thee->ncalc)++;
02779
02780 /* Copy over contents of ELEC */
02781 Nosh_calc_copy(calc, elec);
02782
02783 return 1;
02784 }
02785
02786 VPRIVATE int Nosh_setupCalcPBSAMAUTO(
02787     Nosh *thee,
02788     Nosh_calc *elec
02789 ) {
02790
02791     PBAMParm *parm = VNULL;
02792     PBSAMParm *samparm = VNULL;
02793     PBEParm *pbeparm = VNULL;
02794     Nosh_calc *calc = VNULL;
02795
02796     if (thee == VNULL) {
02797         Vnm_print(2, "Nosh_setupCalcPBSAMAUTO: Got NULL thee!\n");
02798         return 0;
02799     }
02800     if (elec == VNULL) {
02801         Vnm_print(2, "Nosh_setupCalcPBSAMAUTO: Got NULL calc!\n");
02802         return 0;
02803     }
02804     parm = elec->pbamparm;
02805     if (parm == VNULL) {
02806         Vnm_print(2, "Nosh_setupCalcPBSAMAUTO: Got NULL pbamparm -- was this calculation \
02807 set up?\n");
02808         return 0;
02809     }
02810     samparm = elec->pbsamparm;
02811     if (samparm == VNULL) {
02812         Vnm_print(2, "Nosh_setupCalcPBSAMAUTO: Got NULL pbsamparm -- was this calculation \
02813 set up?\n");
02814         return 0;
02815     }
02816     pbeparm = elec->pbeparm;
02817     if (pbeparm == VNULL) {
02818         Vnm_print(2, "Nosh_setupCalcPBSAMAUTO: Got NULL pbeparm -- was this calculation \
02819 set up?\n");
02820         return 0;
02821     }
02822
02823 /* Check to see if he have any room left for this type of calculation, if
02824    so: set the calculation type, update the number of calculations of this type,
02825    and parse the rest of the section */
02826 if (thee->ncalc >= NOSH_MAXCALC) {
02827     Vnm_print(2, "Nosh: Too many calculations in this run!\n");
02828     Vnm_print(2, "Nosh: Current max is %d; ignoring this calculation\n",
02829             NOSH_MAXCALC);
02830     return 0;
02831 }
02832
02833 /* Get the next calculation object and increment the number of calculations */
02834 thee->calc[thee->ncalc] = Nosh_calc_ctor(NCT_PBSAM);
02835 calc = thee->calc[thee->ncalc];
02836 (thee->ncalc)++;
02837
02838 /* Copy over contents of ELEC */
02839 Nosh_calc_copy(calc, elec);
02840
02841 return 1;
02842 }

```

```

02843
02844
02845 VPUBLIC int NOsh_parseBEM(
02846     NOsh *thee,
02847     Vio *sock,
02848     NOsh_calc *elec
02849 ) {
02850
02851     char tok[VMAX_BUFSIZE];
02852     BEMparm *bemparm = VNULL;
02853     PBEParm *pbeparm = VNULL;
02854     int rc;
02855
02856     /* Check the arguments */
02857     if (thee == VNULL) {
02858         Vnm_print(2, "NOsh: Got NULL thee!\n");
02859         return 0;
02860     }
02861     if (sock == VNULL) {
02862         Vnm_print(2, "NOsh: Got pointer to NULL socket!\n");
02863         return 0;
02864     }
02865     if (elec == VNULL) {
02866         Vnm_print(2, "NOsh: Got pointer to NULL elec object!\n");
02867         return 0;
02868     }
02869     bemparm = elec->bemparm;
02870     if (bemparm == VNULL) {
02871         Vnm_print(2, "NOsh: Got pointer to NULL bemparm object!\n");
02872         return 0;
02873     }
02874     pbeparm = elec->pbeparm;
02875     if (pbeparm == VNULL) {
02876         Vnm_print(2, "NOsh: Got pointer to NULL pbeparm object!\n");
02877         return 0;
02878     }
02879
02880     Vnm_print(0, "NOsh_parseBEM: Parsing parameters for BEM calculation\n");
02881
02882     /* Start snarfing tokens from the input stream */
02883     rc = 1;
02884     while (Vio_scanf(sock, "%s", tok) == 1) {
02885
02886         Vnm_print(0, "NOsh_parseBEM: Parsing %s...\n", tok);
02887
02888         /* See if it's an END token */
02889         if (Vstring_strcasecmp(tok, "end") == 0) {
02890             bemparm->parsed = 1;
02891             pbeparm->parsed = 1;
02892             rc = 1;
02893             break;
02894         }
02895     }
02896
02897     /* Pass the token through a series of parsers */
02898     rc = PBEParm_parseToken(pbeparm, tok, sock);
02899     if (rc == -1) {
02900         Vnm_print(0, "NOsh_parseBEM: parsePBE error!\n");
02901         break;
02902     } else if (rc == 0) {
02903         /* Pass the token to the generic BEM parser */
02904         rc = BEMparm_parseToken(bemparm, tok, sock);
02905         if (rc == -1) {
02906             Vnm_print(0, "NOsh_parseBEM: parseBEM error!\n");
02907             break;
02908         } else if (rc == 0) {
02909             /* We ran out of parsers! */
02910             Vnm_print(2, "NOsh: Unrecognized keyword: %s\n", tok);
02911             break;
02912         }
02913     }
02914 }
02915
02916 pbeparm->setsrfm=1;    // unneeded srfm
02917 pbeparm->setpbetype=1; // unneeded pbe type
02918 pbeparm->setbcfl=1;    // unneeded bcfl
02919
02920 /* Handle various errors arising in the token-snarfing loop -- these all
02921    just result in simple returns right now */
02922 if (rc == -1) return 0;
02923 if (rc == 0) return 0;

```

```

02924
02925     /* Check the status of the parameter objects */
02926     if ((BEMparm_check(bemparm) == VRC_FAILURE) || (!PBEParm_check(pbeparm))) {
02927         Vnm_print(2, "Nosh: BEM parameters not set correctly!\n");
02928         return 0;
02929     }
02930
02931     return 1;
02932 }
02933
02934 VPUBLIC int Nosh_parseGEOFLOW(
02935     Nosh *thee,
02936     Vio *sock,
02937     Nosh_calc *elec
02938 ) {
02939
02940     char tok[VMAX_BUFSIZE];
02941     GEOFLOWparm *parm = VNULL;
02942     APOLparm *apolparm = VNULL;
02943     PBEParm *pbeparm = VNULL;
02944     int rc;
02945
02946     /* Check the arguments */
02947     if (thee == VNULL) {
02948         Vnm_print(2, "Nosh: Got NULL thee!\n");
02949         return 0;
02950     }
02951     if (sock == VNULL) {
02952         Vnm_print(2, "Nosh: Got pointer to NULL socket!\n");
02953         return 0;
02954     }
02955     if (elec == VNULL) {
02956         Vnm_print(2, "Nosh: Got pointer to NULL elec object!\n");
02957         return 0;
02958     }
02959     parm = elec->geoflowparm;
02960     if (parm == VNULL) {
02961         Vnm_print(2, "Nosh: Got pointer to NULL geoflowparm object!\n");
02962         return 0;
02963     }
02964     apolparm = elec->apolparm;
02965     if (apolparm == VNULL) {
02966         Vnm_print(2, "Nosh: Got pointer to NULL apolparm object!\n");
02967         return 0;
02968     }
02969     pbeparm = elec->pbeparm;
02970     if (pbeparm == VNULL) {
02971         Vnm_print(2, "Nosh: Got pointer to NULL pbeparm object!\n");
02972         return 0;
02973     }
02974
02975     Vnm_print(0, "Nosh_parseGEOFLOW: Parsing parameters for GEOFLOW calculation\n");
02976
02977     /* Start snarfing tokens from the input stream */
02978     rc = 1;
02979     while (Vio_scanf(sock, "%s", tok) == 1) {
02980
02981         Vnm_print(0, "Nosh_parseGEOFLOW: Parsing %s...\n", tok);
02982
02983         /* See if it's an END token */
02984         if (Vstring_strcasecmp(tok, "end") == 0) {
02985             parm->parsed = 1;
02986             pbeparm->parsed = 1;
02987             apolparm->parsed = 1;
02988             rc = 1;
02989             break;
02990         }
02991
02992         if (Vstring_strcasecmp(tok, "ion") == 0) {
02993             Vnm_print(2, "parseGEOFLOW: WARNING! ion not implemented for geometric flow!\n");
02994         }
02995
02996         /* Pass the token through a series of parsers */
02997         rc = PBEParm_parseToken(pbeparm, tok, sock);
02998         if (rc == -1) {
02999             Vnm_print(0, "Nosh_parseGEOFLOW: parsePBE error!\n");
03000             break;
03001         } else if (rc == 0) {
03002             /* Pass the token to the generic GEOFLOW parser */
03003             rc = APOLparm_parseToken(apolparm, tok, sock);
03004

```

```

03005         if (rc == -1) {
03006             Vnm_print(0, "Nosh_parseAPOL: parseAPOL error!\n");
03007             break;
03008         } else if (rc == 0) {
03009             rc = GEOFLOWparam_parseToken(parm, tok, sock);
03010             if (rc == -1) {
03011                 Vnm_print(0, "Nosh_parseGEOFLOW: parseGEOFLOW error!\n");
03012                 break;
03013             } else if (rc == 0) {
03014                 /* We ran out of parsers! */
03015                 Vnm_print(2, "Nosh: Unrecognized keyword: %s\n", tok);
03016                 break;
03017             }
03018         }
03019     }
03020 }
03021
03022 pbeparm->setsrfm=1;
03023 pbeparm->srاد=0.0;
03024 pbeparm->setsrad=1;
03025 pbeparm->settemp=1;
03026
03027 /* Handle various errors arising in the token-snarfing loop -- these all
03028    just result in simple returns right now */
03029 if (rc == -1) return 0;
03030 if (rc == 0) return 0;
03031
03032 /* Check the status of the parameter objects */
03033 if ((GEOFLOWparam_check(parm) == VRC_FAILURE) || (!PBeparm_check(pbeparm))) {
03034     Vnm_print(2, "Nosh: GEOFLOW parameters not set correctly!\n");
03035     return 0;
03036 }
03037 /*currently the only bc handle by geoflow is mdh so we check here if mdh was read*/
03038 if(pbeparm->bcfl != BCFL_MDH){
03039     Vnm_print(2, "Nosh_parseGEOFLOW: Geoflow currently only supports mdh boundary conditions!\n");
03040     Vnm_print(2, "Nosh_parseGEOFLOW: please change bcfl keyword.\n");
03041     return 0;
03042 }
03043
03044 return 1;
03045 }
03046
03047
03048 VPUBLIC int Nosh_parsePBAM(
03049     Nosh *thee,
03050     Vio *sock,
03051     Nosh_calc *elec
03052 ) {
03053
03054     char tok[VMAX_BUFSIZE];
03055     PBAMparam *parm = VNULL;
03056     PBeparm *pbeparm = VNULL;
03057     int rc;
03058
03059     /* Check the arguments */
03060     if (thee == VNULL) {
03061         Vnm_print(2, "Nosh: Got NULL thee!\n");
03062         return 0;
03063     }
03064     if (sock == VNULL) {
03065         Vnm_print(2, "Nosh: Got pointer to NULL socket!\n");
03066         return 0;
03067     }
03068     if (elec == VNULL) {
03069         Vnm_print(2, "Nosh: Got pointer to NULL elec object!\n");
03070         return 0;
03071     }
03072     parm = elec->pbamparm;
03073     if (parm == VNULL) {
03074         Vnm_print(2, "Nosh: Got pointer to NULL pbam object!\n");
03075         return 0;
03076     }
03077     pbeparm = elec->pbeparm;
03078     if (pbeparm == VNULL) {
03079         Vnm_print(2, "Nosh: Got pointer to NULL pbeparm object!\n");
03080         return 0;
03081     }
03082     Vnm_print(0, "Nosh_parsePBAM: Parsing parameters for PBAM calculation\n");
03083
03084     /* Start snarfing tokens from the input stream */
03085     rc = 1;

```

```

03086     while (Vio_scanf(sock, "%s", tok) == 1) {
03087
03088         Vnm_print(0, "Nosh_parsePBAM: Parsing %s...\n", tok);
03089
03090         /* See if it's an END token */
03091         if (Vstring_strcasecmp(tok, "end") == 0) {
03092             parm->parsed = 1;
03093             pbeparm->parsed = 1;
03094             rc = 1;
03095             break;
03096         }
03097
03098         if (Vstring_strcasecmp(tok, "ion") == 0) {
03099             Vnm_print(2, "parsePBAM: WARNING! PBAM only uses the conc parameter of ion!\n");
03100         }
03101
03102         /* Pass the token through a series of parsers */
03103         rc = PBEParm_parseToken(pbeparm, tok, sock);
03104         if (rc == -1) {
03105             Vnm_print(0, "Nosh_parsePBAM: parsePBE error!\n");
03106             break;
03107         } else if (rc == 0) {
03108             rc = PBAMparm_parseToken(parm, tok, sock);
03109             if (rc == -1) {
03110                 Vnm_print(0, "Nosh_parsePBAM: parsePBAM error!\n");
03111                 break;
03112             } else if (rc == 0) {
03113                 /* We ran out of parsers! */
03114                 Vnm_print(2, "Nosh: Unrecognized keyword: %s\n", tok);
03115                 break;
03116             }
03117         }
03118     }
03119
03120
03121
03122     pbeparm->setsrfm=1;
03123     pbeparm->setsrad=1;
03124     pbeparm->settemp=1; // do need temp, but have default, incase
03125     pbeparm->setmolid=1; // for unneeded mol flag
03126     pbeparm->setpbetype=1; // unneeded pbe type
03127     pbeparm->setbcfl=1; // unneeded bcfl
03128     pbeparm->setsdens=1;
03129
03130     //This is a hacky fix at best for issue 501. This is so we don't need to change PBAM's
03131     //external code.
03132     if (pbeparm->setnion) {
03133         parm->salt = pbeparm->ionc[pbeparm->nion-1];
03134         parm->setsalt = 1;
03135     }
03136
03137     //This is also a hacky fix for issue 488
03138     if (pbeparm->writefmt[pbeparm->numwrite - 1] == VDF_DX) {
03139         strncpy(parm->dxname, pbeparm->writestem[pbeparm->numwrite - 1], CHR_MAXLEN);
03140         parm->setdxname = 1;
03141     }
03142     else {
03143         Vnm_print(2, "Nosh: PBAM only prints in dx format!\n");
03144         return 0;
03145     }
03146
03147     //Another hacky fix for issue 482
03148     if (pbeparm->pbam_3dmapflag == 1) {
03149         strcpy(parm->map3dname, pbeparm->pbam_3dmapstem);
03150         parm->set3dmap = 1;
03151     }
03152
03153     /* Handle various errors arising in the token-snarfing loop -- these all
03154        just result in simple returns right now */
03155     if (rc == -1) return 0;
03156     if (rc == 0) return 0;
03157
03158     /* Check the status of the parameter objects */
03159     if ((PBAMparm_check(parm) == VRC_FAILURE) || (!PBEParm_check(pbeparm))) {
03160         Vnm_print(2, "Nosh: PBAM parameters not set correctly!\n");
03161         return 0;
03162     }
03163     return 1;
03164 }
03165
03166 VPUBLIC int Nosh_parsePBSAM(

```

```

03167             NOsh *thee,
03168             Vio *sock,
03169             NOsh_calc *elec
03170         ) {
03171
03172         char tok[VMAX_BUFSIZE];
03173         PBAMparm *parm = VNULL;
03174         PBSAMparm *samparm = VNULL;
03175         PBEParm *pbeparm = VNULL;
03176         int rc;
03177
03178         /* Check the arguments */
03179         if (thee == VNULL) {
03180             Vnm_print(2, "NOsh: Got NULL thee!\n");
03181             return 0;
03182         }
03183         if (sock == VNULL) {
03184             Vnm_print(2, "NOsh: Got pointer to NULL socket!\n");
03185             return 0;
03186         }
03187         if (elec == VNULL) {
03188             Vnm_print(2, "NOsh: Got pointer to NULL elec object!\n");
03189             return 0;
03190         }
03191         parm = elec->pbamparm;
03192         if (parm == VNULL) {
03193             Vnm_print(2, "NOsh: Got pointer to NULL pbam object!\n");
03194             return 0;
03195         }
03196         samparm = elec->pbsamparm;
03197         if (samparm == VNULL) {
03198             Vnm_print(2, "NOsh: Got pointer to NULL pbsam object!\n");
03199             return 0;
03200         }
03201         pbeparm = elec->pbeparm;
03202         if (pbeparm == VNULL) {
03203             Vnm_print(2, "NOsh: Got pointer to NULL pbeparm object!\n");
03204             return 0;
03205         }
03206         Vnm_print(0, "NOsh_parsePBSAM: Parsing parameters for PBSAM calculation\n");
03207
03208         /* Start snarfing tokens from the input stream */
03209         rc = 1;
03210         while (Vio_scanf(sock, "%s", tok) == 1) {
03211
03212             Vnm_print(0, "NOsh_parsePBSAM: Parsing %s...\n", tok);
03213
03214             /* See if it's an END token */
03215             if (Vstring_strcasecmp(tok, "end") == 0) {
03216                 parm->parsed = 1;
03217                 samparm->parsed = 1;
03218                 pbeparm->parsed = 1;
03219                 rc = 1;
03220                 break;
03221             }
03222
03223             if (Vstring_strcasecmp(tok, "ion") == 0) {
03224                 Vnm_print(2, "parsePBSAM: WARNING! PBAM only uses the conc parameter of ion!\n");
03225             }
03226
03227             /* Pass the token through a series of parsers */
03228             rc = PBEParm_parseToken(pbeparm, tok, sock);
03229             if (rc == -1) {
03230                 Vnm_print(0, "NOsh_parsePBSAM: parsePBE error!\n");
03231                 break;
03232             } else if (rc == 0) {
03233                 rc = PBAMparm_parseToken(parm, tok, sock);
03234                 if (rc == -1) {
03235                     Vnm_print(0, "NOsh_parsePBSAM: parsePBAM error!\n");
03236                     break;
03237                 } else if (rc == 0) {
03238                     rc = PBSAMparm_parseToken(samparm, tok, sock);
03239                     if (rc == -1) {
03240                         Vnm_print(0, "NOsh_parsePBSAM: parsePBSAM error!\n");
03241                         break;
03242                     } else if (rc == 0) {
03243                         /* We ran out of parsers! */
03244                         Vnm_print(2, "NOsh: Unrecognized keyword: %s\n", tok);
03245                         break;
03246                     }
03247                 }
03248             }
03249         }

```

```

03248     }
03249 }
03250
03251 pbeparm->setsrfm=1;
03252 pbeparm->setsrad=1;
03253 pbeparm->settemp=1; // do need temp, but have default, incase
03254 pbeparm->setmolid=1; // for unneeded mol flag
03255 pbeparm->setpbetype=1; // unneeded pbe type
03256 pbeparm->setbcfl=1; // unneeded bcfl
03257 pbeparm->setsdens=1;
03258
03259 //This is a hacky fix at best for issue 501. This is so we don't need to change PBAM's
03260 //external code.
03261 if (pbeparm->setnion) {
03262     parm->salt = pbeparm->ionc[pbeparm->nion-1];
03263     parm->setsalt = 1;
03264 }
03265
03266 //This is also a hacky fix for issue 488
03267 if (pbeparm->writefmt[pbeparm->numwrite - 1] == VDF_DX) {
03268     strncpy(parm->dxname, pbeparm->writestem[pbeparm->numwrite - 1], CHR_MAXLEN);
03269     parm->setdxname = 1;
03270 }
03271 else {
03272     Vnm_print(2, "Nosh: PBSAM only prints in dx format!\n");
03273     return 0;
03274 }
03275
03276
03277 /* Handle various errors arising in the token-snarfing loop -- these all
03278    just result in simple returns right now */
03279 if (rc == -1) return 0;
03280 if (rc == 0) return 0;
03281
03282 /* Check the status of the parameter objects */
03283 if ((PBSAMparm_check(samparm) == VRC_FAILURE) ||
03284     (PBAMparm_check(parm) == VRC_FAILURE) ||
03285     (!PBEParm_check(pbeparm))) {
03286     Vnm_print(2, "Nosh: PBSAM parameters not set correctly!\n");
03287     return 0;
03288 }
03289 return 1;
03290 }

```

9.36 src/generic/nosh.h File Reference

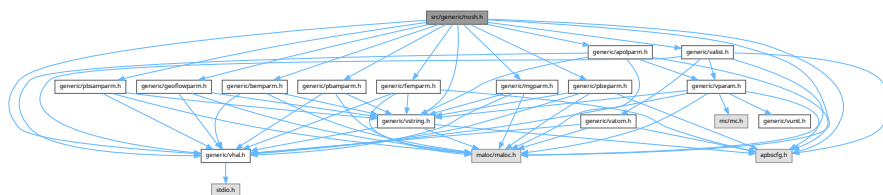
Contains declarations for class NOsh.

```

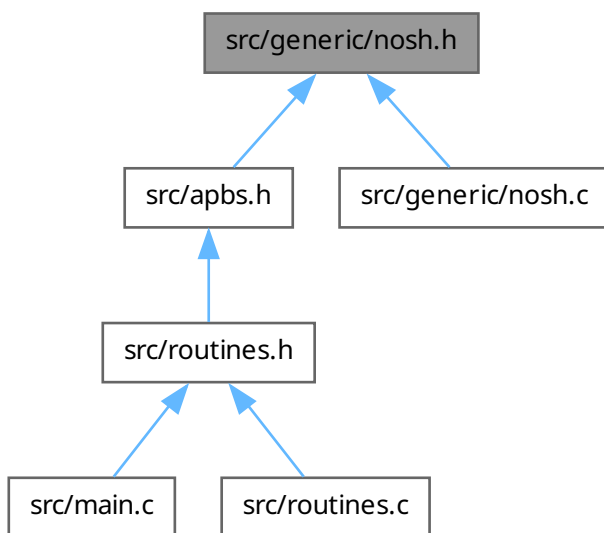
#include "apbscfg.h"
#include "malloc/malloc.h"
#include "generic/vhal.h"
#include "generic/vstring.h"
#include "generic/pbeparm.h"
#include "generic/mgparm.h"
#include "generic/apolparm.h"
#include "generic/femparm.h"
#include "generic/valist.h"
#include "generic/bemparm.h"
#include "generic/geoflowparm.h"
#include "generic/pbamparm.h"
#include "generic/pbsamparm.h"

```

Include dependency graph for nosh.h:



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [sNOsh_calc](#)
Calculation class for use when parsing fixed format input files.
- struct [sNOsh](#)
Class for parsing fixed format input files.

Macros

- #define [NOSH_MAXMOL](#) 20
Maximum number of molecules in a run.
- #define [NOSH_MAXCALC](#) 20
Maximum number of calculations in a run.
- #define [NOSH_MAXPRINT](#) 20
Maximum number of PRINT statements in a run.

- #define `NOSH_MAXPOP` 20
Maximum number of operations in a PRINT statement.

Typedefs

- typedef enum `eNosh_MolFormat` `Nosh_MolFormat`
Declare Nosh_MolFormat type.
- typedef enum `eNosh_CalcType` `Nosh_CalcType`
Declare Nosh_CalcType type.
- typedef enum `eNosh_ParmFormat` `Nosh_ParmFormat`
Declare Nosh_ParmFormat type.
- typedef enum `eNosh_PrintType` `Nosh_PrintType`
Declare Nosh_PrintType type.
- typedef struct `sNosh_calc` `Nosh_calc`
- typedef struct `sNosh` `Nosh`
Declaration of the Nosh class as the Nosh structure.

Enumerations

- enum `eNosh_MolFormat` { `NMF_PQR` =0 , `NMF_PDB` =1 , `NMF_XML` =2 }
Molecule file format types.
- enum `eNosh_CalcType` {
`NCT_MG` =0 , `NCT_FEM` =1 , `NCT_APOL` =2 , `NCT_BEM` =3 ,
`NCT_GEOFLOW` =4 , `NCT_PBAM` =5 , `NCT_PBSAM` =6 }
Nosh calculation types.
- enum `eNosh_ParmFormat` { `NPF_FLAT` =0 , `NPF_XML` =1 }
Parameter file format types.
- enum `eNosh_PrintType` {
`NPT_ENERGY` =0 , `NPT_FORCE` =1 , `NPT_ELECENERGY` , `NPT_ELECFORCE` ,
`NPT_APOLENERGY` , `NPT_APOLFORCE` }
Nosh print types.

Functions

- VEXTERNC char * `Nosh_getMolpath` (`Nosh` *thee, int imol)
Returns path to specified molecule.
- VEXTERNC char * `Nosh_getDielXpath` (`Nosh` *thee, int imap)
Returns path to specified x-shifted dielectric map.
- VEXTERNC char * `Nosh_getDielYpath` (`Nosh` *thee, int imap)
Returns path to specified y-shifted dielectric map.
- VEXTERNC char * `Nosh_getDielZpath` (`Nosh` *thee, int imap)
Returns path to specified z-shifted dielectric map.
- VEXTERNC char * `Nosh_getKappapath` (`Nosh` *thee, int imap)
Returns path to specified kappa map.
- VEXTERNC char * `Nosh_getPotpath` (`Nosh` *thee, int imap)
Returns path to specified potential map.
- VEXTERNC char * `Nosh_getChargepath` (`Nosh` *thee, int imap)
Returns path to specified charge distribution map.
- VEXTERNC `Nosh_calc` * `Nosh_getCalc` (`Nosh` *thee, int icalc)

- Returns specified calculation object.*

 - VEXTERNC int [NOsh_getDielfmt](#) ([NOsh](#) *thee, int imap)

Returns format of specified dielectric map.
- VEXTERNC int [NOsh_getKappafmt](#) ([NOsh](#) *thee, int imap)

Returns format of specified kappa map.
- VEXTERNC int [NOsh_getPotfmt](#) ([NOsh](#) *thee, int imap)

Returns format of specified potential map.
- VEXTERNC int [NOsh_getChargefmt](#) ([NOsh](#) *thee, int imap)

Returns format of specified charge map.
- VEXTERNC [NOsh_PrintType](#) [NOsh_printWhat](#) ([NOsh](#) *thee, int iprint)

Return an integer ID of the observable to print (.
- VEXTERNC char * [NOsh_elecname](#) ([NOsh](#) *thee, int ielec)

Return an integer mapping of an ELEC statement to a calculation ID (.
- VEXTERNC int [NOsh_elec2calc](#) ([NOsh](#) *thee, int icalc)

Return the name of an elec statement.
- VEXTERNC int [NOsh_apol2calc](#) ([NOsh](#) *thee, int icalc)

Return the name of an apol statement.
- VEXTERNC int [NOsh_printNarg](#) ([NOsh](#) *thee, int iprint)

Return number of arguments to PRINT statement (.
- VEXTERNC int [NOsh_printOp](#) ([NOsh](#) *thee, int iprint, int iarg)

Return integer ID for specified operation (.
- VEXTERNC int [NOsh_printCalc](#) ([NOsh](#) *thee, int iprint, int iarg)

Return calculation ID for specified PRINT statement (.
- VEXTERNC [NOsh](#) * [NOsh_ctor](#) (int rank, int size)

Construct NOsh.
- VEXTERNC [NOsh_calc](#) * [NOsh_calc_ctor](#) ([NOsh_CalcType](#) calcType)

Construct NOsh_calc.
- VEXTERNC int [NOsh_calc_copy](#) ([NOsh_calc](#) *thee, [NOsh_calc](#) *source)

Copy NOsh_calc object into thee.
- VEXTERNC void [NOsh_calc_dtor](#) ([NOsh_calc](#) **thee)

Object destructor.
- VEXTERNC int [NOsh_ctor2](#) ([NOsh](#) *thee, int rank, int size)

FORTTRAN stub to construct NOsh.
- VEXTERNC void [NOsh_dtor](#) ([NOsh](#) **thee)

Object destructor.
- VEXTERNC void [NOsh_dtor2](#) ([NOsh](#) *thee)

FORTTRAN stub for object destructor.
- VEXTERNC int [NOsh_parseInput](#) ([NOsh](#) *thee, Vio *sock)

Parse an input file from a socket.
- VEXTERNC int [NOsh_parseInputFile](#) ([NOsh](#) *thee, char *filename)

Parse an input file only from a file.
- VEXTERNC int [NOsh_setupElecCalc](#) ([NOsh](#) *thee, [Valist](#) *alist[[NOSH_MAXMOL](#)])

Setup the series of electrostatics calculations.
- VEXTERNC int [NOsh_setupApolCalc](#) ([NOsh](#) *thee, [Valist](#) *alist[[NOSH_MAXMOL](#)])

Setup the series of non-polar calculations.

9.36.1 Detailed Description

Contains declarations for class NOsh.

Version

\$Id\$

Author

Nathan A. Baker

Attention

```
*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
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*   Pacific Northwest National Laboratory
*
*   Additional contributing authors listed in the code documentation.
*
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* THE POSSIBILITY OF SUCH DAMAGE.
*
*
```

Definition in file [nosh.h](#).

9.36.2 Typedef Documentation

9.36.2.1 NOsh_calc

```
typedef struct sNOsh_calc NOsh_calc
```

Definition at line 188 of file [nosh.h](#).

9.37 nosh.h

[Go to the documentation of this file.](#)

```

00001
00062 #ifndef _NOSH_H_
00063 #define _NOSH_H_
00064
00065 #include "apbscfg.h"
00066
00067 #include "malloc/malloc.h"
00068
00069 #include "generic/vhal.h"
00070 #include "generic/vstring.h"
00071 #include "generic/pbeparm.h"
00072 #include "generic/mgparm.h"
00073 #include "generic/apolparm.h"
00074 #include "generic/femparm.h"
00075 #include "generic/valist.h"
00076 #include "generic/bemparm.h"
00077 #include "generic/geoflowparm.h"
00078 #include "generic/pbamparm.h"
00079 #include "generic/pbsamparm.h" //path might change
00080
00083 #define NOSH_MAXMOL 20
00084
00087 #define NOSH_MAXCALC 20
00088
00091 #define NOSH_MAXPRINT 20
00092
00095 #define NOSH_MAXPOP 20
00096
00101 enum eNosh_MolFormat {
00102     NMF_PQR=0,
00103     NMF_PDB=1,
00104     NMF_XML=2
00105 };
00106
00111 typedef enum eNosh_MolFormat Nosh_MolFormat;
00112
00117 enum eNosh_CalcType {
00118     NCT_MG=0,
00119     NCT_FEM=1,
00120     NCT_APOL=2,
00121     NCT_BEM=3,
00122     NCT_GEOFLOW=4,
00123     NCT_PBAM=5,
00124     NCT_PBSAM=6
00125 };
00126
00131 typedef enum eNosh_CalcType Nosh_CalcType;
00132
00137 enum eNosh_ParmFormat {
00138     NPF_FLAT=0,
00139     NPF_XML=1
00140 };
00141
00146 typedef enum eNosh_ParmFormat Nosh_ParmFormat;
00147
00152 enum eNosh_PrintType {
00153     NPT_ENERGY=0,
00154     NPT_FORCE=1,
00155     NPT_ELECENERGY,
00156     NPT_ELECFORCE,
00157     NPT_APOLENERGY,
00158     NPT_APOLFORCE
00159 };
00160
00165 typedef enum eNosh_PrintType Nosh_PrintType;
00166
00172 struct sNosh_calc {
00173     MGparm *mgparm;
00174     FEMparm *femparm;
00175     BEMparm *bemparm;
00176     GEOFLOWparm *geoflowparm;
00177     PBAMparm *pbamparm;
00178     PBSAMparm *pbsamparm;

```

```

00179     PBEparm *pbeparm;
00180     APOLparm *apolparm;
00181     NOsh_CalcType calctype;
00182 };
00183
00188 typedef struct sNOsh_calc NOsh_calc;
00189
00195 struct sNOsh {
00196
00197     NOsh_calc *calc[NOSH_MAXCALC];
00200     int ncalc;
00202     NOsh_calc *elec[NOSH_MAXCALC];
00205     int nelec;
00208     NOsh_calc *apol[NOSH_MAXCALC];
00211     int napol;
00214     int ispara;
00215     int proc_rank;
00216     int proc_size;
00217     int bogus;
00221     int elec2calc[NOSH_MAXCALC];
00229     int apol2calc[NOSH_MAXCALC];
00231     int nmol;
00232     char molpath[NOSH_MAXMOL][VMAX_ARGLEN];
00233     NOsh_MolFormat molfmt[NOSH_MAXMOL];
00234     Valist *alist[NOSH_MAXMOL];
00236     int gotparm;
00237     char parmpath[VMAX_ARGLEN];
00238     NOsh_ParmFormat parmfmt;
00239     int ndiel;
00240     char dielXpath[NOSH_MAXMOL][VMAX_ARGLEN];
00242     char dielYpath[NOSH_MAXMOL][VMAX_ARGLEN];
00244     char dielZpath[NOSH_MAXMOL][VMAX_ARGLEN];
00246     Vdata_Format dielfmt[NOSH_MAXMOL];
00247     int nkappa;
00248     char kappapath[NOSH_MAXMOL][VMAX_ARGLEN];
00249     Vdata_Format kappafmt[NOSH_MAXMOL];
00250     int npot;
00251     char potpath[NOSH_MAXMOL][VMAX_ARGLEN];
00252     Vdata_Format potfmt[NOSH_MAXMOL];
00253     int ncharge;
00254     char chargepath[NOSH_MAXMOL][VMAX_ARGLEN];
00255     Vdata_Format chargefmt[NOSH_MAXMOL];
00256     int nmesh;
00257     char meshpath[NOSH_MAXMOL][VMAX_ARGLEN];
00258     Vdata_Format meshfmt[NOSH_MAXMOL];
00259     int nprint;
00260     NOsh_PrintType printwhat[NOSH_MAXPRINT];
00262     int printnarg[NOSH_MAXPRINT];
00263     int printcalc[NOSH_MAXPRINT][NOSH_MAXPOP];
00264     int printop[NOSH_MAXPRINT][NOSH_MAXPOP];
00266     int parsed;
00267     char elecname[NOSH_MAXCALC][VMAX_ARGLEN];
00269     char apolname[NOSH_MAXCALC][VMAX_ARGLEN];
00271 };
00272
00277 typedef struct sNOsh NOsh;
00278
00279 /* ////////////////////////////////////////
00280 // Class NOsh: Inlineable methods (mcsh.c)
00282 #if !defined(VINLINE_NOSH)
00290 VEXTERNC char* NOsh_getMolpath(NOsh *thee, int imol);
00291
00299 VEXTERNC char* NOsh_getDielXpath(NOsh *thee, int imap);
00300
00308 VEXTERNC char* NOsh_getDielYpath(NOsh *thee, int imap);
00309
00317 VEXTERNC char* NOsh_getDielZpath(NOsh *thee, int imap);
00318
00326 VEXTERNC char* NOsh_getKappapath(NOsh *thee, int imap);
00327
00335 VEXTERNC char* NOsh_getPotpath(NOsh *thee, int imap);
00336
00344 VEXTERNC char* NOsh_getChargepath(NOsh *thee, int imap);
00345
00353 VEXTERNC NOsh_calc* NOsh_getCalc(NOsh *thee, int icalc);
00354
00362 VEXTERNC int NOsh_getDielfmt(NOsh *thee, int imap);
00363
00371 VEXTERNC int NOsh_getKappafmt(NOsh *thee, int imap);
00372
00380 VEXTERNC int NOsh_getPotfmt(NOsh *thee, int imap);

```

```

00381
00389 VEXTERNC int NOsh_getChargefmt(NOsh *thee, int imap);
00390
00391 #else
00392
00393 #   define NOsh_getMolpath(thee, imol) ((thee)->molpath[(imol)])
00394 #   define NOsh_getDielXpath(thee, imol) ((thee)->dielXpath[(imol)])
00395 #   define NOsh_getDielYpath(thee, imol) ((thee)->dielYpath[(imol)])
00396 #   define NOsh_getDielZpath(thee, imol) ((thee)->dielZpath[(imol)])
00397 #   define NOsh_getKappapath(thee, imol) ((thee)->kappapath[(imol)])
00398 #   define NOsh_getPotpath(thee, imol) ((thee)->potpath[(imol)])
00399 #   define NOsh_getChargepath(thee, imol) ((thee)->chargepath[(imol)])
00400 #   define NOsh_getCalc(thee, icalc) ((thee)->calc[(icalc)])
00401 #   define NOsh_getDielfmt(thee, imap) ((thee)->dielfmt[(imap)])
00402 #   define NOsh_getKappafmt(thee, imap) ((thee)->kappafmt[(imap)])
00403 #   define NOsh_getPotfmt(thee, imap) ((thee)->potfmt[(imap)])
00404 #   define NOsh_getChargefmt(thee, imap) ((thee)->chargefmt[(imap)])
00405
00406 #endif
00407
00408
00409 /* ////////////////////////////////////////
00410    // Class NOsh: Non-inlineable methods (mcsh.c)
00411    ////////////////////////////////////////
00412
00420 VEXTERNC NOsh_PrintType NOsh_printWhat(NOsh *thee, int iprint);
00421
00431 VEXTERNC char* NOsh_elecname(NOsh *thee, int ielec);
00432
00440 VEXTERNC int NOsh_elec2calc(NOsh *thee, int icalc);
00441
00449 VEXTERNC int NOsh_apol2calc(NOsh *thee, int icalc);
00450
00458 VEXTERNC int NOsh_printNarg(NOsh *thee, int iprint);
00459
00468 VEXTERNC int NOsh_printOp(NOsh *thee, int iprint, int iarg);
00469
00480 VEXTERNC int NOsh_printCalc(NOsh *thee, int iprint, int iarg);
00481
00491 VEXTERNC NOsh* NOsh_ctor(int rank, int size);
00492
00499 VEXTERNC NOsh_calc* NOsh_calc_ctor(
00500     NOsh_CalcType calcType
00501 );
00502
00509 VEXTERNC int NOsh_calc_copy(
00510     NOsh_calc *thee,
00511     NOsh_calc *source
00512 );
00513
00519 VEXTERNC void NOsh_calc_dtor(NOsh_calc **thee);
00520
00531 VEXTERNC int NOsh_ctor2(NOsh *thee, int rank, int size);
00532
00538 VEXTERNC void NOsh_dtor(NOsh **thee);
00539
00545 VEXTERNC void NOsh_dtor2(NOsh *thee);
00546
00555 VEXTERNC int NOsh_parseInput(NOsh *thee, Vio *sock);
00556
00566 VEXTERNC int NOsh_parseInputFile(NOsh *thee, char *filename);
00567
00577 VEXTERNC int NOsh_setupElecCalc(
00578     NOsh *thee, /**< NOsh object */
00579     Valist *alist[NOSH_MAXMOL]
00580 );
00581
00591 VEXTERNC int NOsh_setupApolCalc(
00592     NOsh *thee,
00593     Valist *alist[NOSH_MAXMOL]
00594 );
00595
00596 #endif
00597

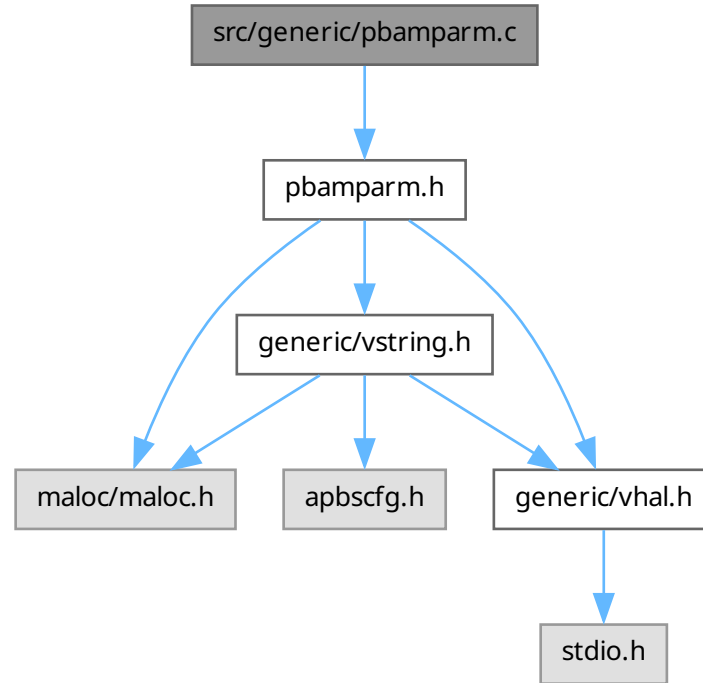
```

9.38 src/generic/pbamparm.c File Reference

Class PBAMparm methods.

```
#include "pbamparm.h"
```

Include dependency graph for pbamparm.c:



Functions

- `VPUBLIC PBAMparm * PBAMparm_ctor (PBAMparm_CalcType type)`
Construct PBAMparm object.
- `VPUBLIC Vrc_Codes PBAMparm_ctor2 (PBAMparm *thee, PBAMparm_CalcType type)`
FORTTRAN stub to construct PBAMparm object ??????????!!!!!!
- `VPUBLIC void PBAMparm_dtor (PBAMparm **thee)`
Object destructor.
- `VPUBLIC void PBAMparm_dtor2 (PBAMparm *thee)`
FORTTRAN stub for object destructor ??????????!!!!!!
- `VPUBLIC Vrc_Codes PBAMparm_check (PBAMparm *thee)`
Consistency check for parameter values stored in object.
- `VPUBLIC void PBAMparm_copy (PBAMparm *thee, PBAMparm *parm)`
copy PBAMparm object int thee.
- `VPRIVATE Vrc_Codes PBAMparm_parseSalt (PBAMparm *thee, Vio *sock)`
Find salt conc and save it as a structure variable.
- `VPRIVATE Vrc_Codes PBAMparm_parseRunType (PBAMparm *thee, Vio *sock)`
Find runType and save it as a structure variable.
- `VPRIVATE Vrc_Codes PBAMparm_parseRunName (PBAMparm *thee, Vio *sock)`

- Find runName and save it as a structure variable.*
- VPRIVATE Vrc_Codes PBAMparm_parseRandorient (PBAMparm *thee, Vio *sock)
 - Find randomorientation flag and save it as a boolean.*
- VPRIVATE Vrc_Codes PBAMparm_parsePBCS (PBAMparm *thee, Vio *sock)
 - Find PBC flag and save the type and the boxlength.*
- VPRIVATE Vrc_Codes PBAMparm_parseUnits (PBAMparm *thee, Vio *sock)
 - Find units flag and save units.*
- VPRIVATE Vrc_Codes PBAMparm_parseGridPts (PBAMparm *thee, Vio *sock)
 - Find Grid points and save them.*
- VPRIVATE Vrc_Codes PBAMparm_parse3Dmap (PBAMparm *thee, Vio *sock)
 - Find 3D map filename and save it.*
- VPRIVATE Vrc_Codes PBAMparm_parseGrid2D (PBAMparm *thee, Vio *sock)
 - Find 2D grid filename and save it.*
- VPRIVATE Vrc_Codes PBAMparm_parseDX (PBAMparm *thee, Vio *sock)
 - Find DX filename and save it.*
- VPRIVATE Vrc_Codes PBAMparm_parseTermcombine (PBAMparm *thee, Vio *sock)
 - Find Termination logic and save it.*
- VPRIVATE Vrc_Codes PBAMparm_parseNtraj (PBAMparm *thee, Vio *sock)
- VPRIVATE Vrc_Codes PBAMparm_parseDiff (PBAMparm *thee, Vio *sock)
 - Find diffusion coeffs for each molecule and save them.*
- VPRIVATE Vrc_Codes PBAMparm_parseTerm (PBAMparm *thee, Vio *sock)
- VPRIVATE Vrc_Codes PBAMparm_parseXYZ (PBAMparm *thee, Vio *sock)
 - Find xyz files for each molecule for each traj and save them.*
- VPUBLIC Vrc_Codes PBAMparm_parseToken (PBAMparm *thee, char tok[VMAX_BUFSIZE], Vio *sock)
 - Parse an MG keyword from an input file.*

9.38.1 Detailed Description

Class PBAMparm methods.

Author

Andrew Stevens

Version

\$Id\$

Attention

```
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* APBS -- Adaptive Poisson-Boltzmann Solver
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*
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* THE POSSIBILITY OF SUCH DAMAGE.
*
*

```

Definition in file [pbamparm.c](#).

9.38.2 Function Documentation

9.38.2.1 PBAMparm_parseNtraj()

```

VPRIVATE Vrc_Codes PBAMparm_parseNtraj (
    PBAMparm * thee,
    Vio * sock )

```

Definition at line 458 of file [pbamparm.c](#).

9.38.2.2 PBAMparm_parseTerm()

```

VPRIVATE Vrc_Codes PBAMparm_parseTerm (
    PBAMparm * thee,
    Vio * sock )

```

Definition at line 549 of file [pbamparm.c](#).

9.39 pbamparm.c

[Go to the documentation of this file.](#)

```

00001
00057 #include "pbamparm.h"
00058
00059 VEMBED(rcsid="$Id$")
00060
00061 #if !defined(VINLINE_MGPARM)
00062
00063 #endif /* if !defined(VINLINE_MGPARM) */
00064
00065
00066 VPUBLIC PBAMparm* PBAMparm_ctor(PBAMparm_CalcType type) {

```

```

00067
00068     /* Set up the structure */
00069     PBAMparm *thee = VNULL;
00070     thee = (PBAMparm*)Vmem_malloc(VNULL, 1, sizeof(PBAMparm));
00071     VASSERT( thee != VNULL);
00072     VASSERT( PBAMparm_ctor2(thee, type) == VRC_SUCCESS );
00073
00074     return thee;
00075 }
00076
00077 VPUBLIC Vrc_Codes PBAMparm_ctor2(PBAMparm *thee, PBAMparm_CalcType type) {
00078
00079     int i;
00080
00081     if (thee == VNULL) return VRC_FAILURE;
00082
00083     thee->parsed = 0;
00084     thee->type = type;
00085     thee->salt = 0;
00086
00087     thee->setsalt = 0;
00088     thee->setruntype = 0;
00089     thee->setrunname = 0;
00090     thee->setunits = 0;
00091
00092     thee->setrandorient = 0;
00093
00094     thee->setpbcs = 0;
00095     thee->pbcbboxlen = 1e15;
00096
00097     // Electrostatics
00098     thee->gridpt = 15;
00099     printf("Found a pts flag in ctor: %d\n", thee->gridpt);
00100     thee->setgridpt = 0;
00101     thee->set3dmap = 0;
00102     thee->setgrid2Dname = 0;
00103     thee->grid2Dct = 0;
00104     thee->setdxname = 0;
00105
00106     //Dynamics
00107     thee->ntraj = 1;
00108     thee->setntraj = 0;
00109
00110     thee->settermcombine = 0;
00111     thee->diffct = 0;
00112
00113     thee->termct = 0;
00114     thee->setterm = 0;
00115
00116     thee->setxyz = 0;
00117     for (i = 0; i<PBAMPARM_MAXMOL; i++) thee->xyzct[i] = 0;
00118
00119     return VRC_SUCCESS;
00120 }
00121
00122 VPUBLIC void PBAMparm_dtor(PBAMparm **thee) {
00123     if ((*thee) != VNULL) {
00124         PBAMparm_dtor2(*thee);
00125         Vmem_free(VNULL, 1, sizeof(PBAMparm), (void **)thee);
00126         (*thee) = VNULL;
00127     }
00128 }
00129
00130 VPUBLIC void PBAMparm_dtor2(PBAMparm *thee) { ; }
00131
00132 VPUBLIC Vrc_Codes PBAMparm_check(PBAMparm *thee) {
00133
00134     Vrc_Codes rc;
00135
00136     rc = VRC_SUCCESS;
00137
00138     Vnm_print(0, "PBAMparm_check:  checking PBAMparm object of type %d.\n",
00139               thee->type);
00140
00141     /* Check to see if we were even filled... */
00142     if (!thee->parsed) {
00143         Vnm_print(2, "PBAMparm_check:  not filled!\n");
00144         return VRC_FAILURE;
00145     }
00146
00147

```

```

00148     /* Check type settings */
00149     if (thee->type != PBAMCT_AUTO) {
00150         Vnm_print(2, "PBAMparm_check: type not set");
00151         rc = VRC_FAILURE;
00152     }
00153
00154     return rc;
00155 }
00156
00157 VPUBLIC void PBAMparm_copy(PBAMparm *thee, PBAMparm *parm) {
00158     int i, j, k;
00159     VASSERT(thee != VNULL);
00160     VASSERT(parm != VNULL);
00161
00162     thee->type = parm->type;
00163     thee->parsed = parm->parsed;
00164
00165     thee->salt = parm->salt;
00166     thee->setsalt = parm->setsalt;
00167     for (i=0; i<CHR_MAXLEN; i++) thee->runtype[i] = parm->runtype[i];
00168     thee->setruntype = parm->setruntype;
00169
00170     for (i=0; i<CHR_MAXLEN; i++) thee->runname[i] = parm->runname[i];
00171     thee->setrunname = parm->setrunname;
00172
00173     thee->setrandorient = parm->setrandorient;
00174
00175     thee->setpbcs = parm->setpbcs;
00176     thee->pbcbboxlen = parm->pbcbboxlen;
00177
00178     for (i=0; i<CHR_MAXLEN; i++) thee->units[i] = parm->units[i];
00179     thee->setunits = parm->setunits;
00180
00181     // Electrostatic parts
00182     thee->gridpt = parm->gridpt;
00183     thee->setgridpt = parm->setgridpt;
00184     for (i=0; i<CHR_MAXLEN; i++) thee->map3dname[i] = parm->map3dname[i];
00185     thee->set3dmap = parm->set3dmap;
00186
00187     thee->grid2Dct = parm->grid2Dct;
00188     for (i=0; i<PBAMPARM_MAXWRITE; i++)
00189     {
00190         for (j=0; j<CHR_MAXLEN; j++)
00191         {
00192             thee->grid2Dname[i][j] = parm->grid2Dname[i][j];
00193             thee->grid2Dax[i][j] = parm->grid2Dax[i][j];
00194         }
00195         thee->grid2Dloc[i] = parm->grid2Dloc[i];
00196     }
00197
00198     for (i=0; i<CHR_MAXLEN; i++) thee->dxname[i] = parm->dxname[i];
00199     thee->setdxname = parm->setdxname;
00200
00201     // Dynamics parts
00202     thee->ntraj = parm->ntraj;
00203     thee->setntraj = parm->setntraj;
00204
00205     for (i=0; i<CHR_MAXLEN; i++) thee->termcombine[i] = parm->termcombine[i];
00206     thee->settermcombine = parm->settermcombine;
00207
00208     thee->diffct = parm->diffct;
00209
00210     for (i=0; i<PBAMPARM_MAXMOL; i++)
00211     {
00212         for (j=0; j<CHR_MAXLEN; j++)
00213         {
00214             thee->moveType[i][j] = parm->moveType[i][j];
00215         }
00216         thee->transDiff[i] = parm->transDiff[i];
00217         thee->rotDiff[i] = parm->rotDiff[i];
00218     }
00219
00220     thee->termct = parm->termct;
00221     thee->setterm = parm->setterm;
00222     thee->confilct = parm->confilct;
00223
00224     for (i=0; i<PBAMPARM_MAXWRITE; i++)
00225     {
00226         for (j=0; j<CHR_MAXLEN; j++)
00227         {

```

```

00229         thee->termnam[i][j] = parm->termnam[i][j];
00230         thee->confil[i][j] = parm->confil[i][j];
00231     }
00232     thee->termVal[i] = parm->termVal[i];
00233     thee->termnu[i][0] = parm->termnu[i][0];
00234 }
00235
00236 thee->setxyz = parm->setxyz;
00237 for (i = 0; i<PBAMPARM_MAXMOL; i++)
00238 {
00239     thee->xyzct[i] = parm->xyzct[i];
00240     for (j = 0; j<PBAMPARM_MAXWRITE; j++)
00241     {
00242         for (k = 0; k<CHR_MAXLEN; k++)
00243         {
00244             thee->xyzfil[i][j][k] = parm->xyzfil[i][j][k];
00245         }
00246     }
00247 }
00248
00249 }
00250
00251
00252 VPRIVATE Vrc_Codes PBAMParm_parseSalt(PBAMParm *thee, Vio *sock){
00253     const char* name = "salt";
00254     char tok[VMAX_BUFSIZE];
00255     double tf;
00256     if(Vio_scanf(sock, "%s", tok) == 0) {
00257         Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00258         return VRC_WARNING;
00259     }
00260
00261     if (sscanf(tok, "%lf", &tf) == 0){
00262         Vnm_print(2, "Nosh: Read non-float (%s) while parsing %s keyword!\n", tok, name);
00263         return VRC_WARNING;
00264     }else{
00265         thee->salt = tf;
00266     }
00267     thee->setsalt = 1;
00268     return VRC_SUCCESS;
00269 }
00270
00271 VPRIVATE Vrc_Codes PBAMParm_parseRunType(PBAMParm *thee, Vio *sock){
00272     const char* name = "runtype";
00273     char tok[VMAX_BUFSIZE];
00274
00275     if(Vio_scanf(sock, "%s", tok) == 0) {
00276         Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00277         return VRC_WARNING;
00278     } else if (Vstring_strcasecmp(tok, "dynamics") == 0){
00279         Vnm_print(2, "parsePBAM: Dynamics has been moved out of the ELEC section!\n");
00280         return VRC_WARNING;
00281     } else {
00282         strncpy(thee->runtype, tok, CHR_MAXLEN);
00283         thee->setruntype=1;
00284     }
00285
00286     return VRC_SUCCESS;
00287 }
00288
00289 VPRIVATE Vrc_Codes PBAMParm_parseRunName(PBAMParm *thee, Vio *sock){
00290     const char* name = "runname";
00291     char tok[VMAX_BUFSIZE];
00292
00293     if(Vio_scanf(sock, "%s", tok) == 0) {
00294         Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00295         return VRC_WARNING;
00296     } else {
00297         strncpy(thee->runname, tok, CHR_MAXLEN);
00298         thee->setrunname=1;
00299     }
00300
00301     return VRC_SUCCESS;
00302 }
00303
00304 VPRIVATE Vrc_Codes PBAMParm_parseRanderient(PBAMParm *thee, Vio *sock){
00305     const char* name = "randerient";
00306     thee->setranderient=1;
00307     return VRC_SUCCESS;
00308 }
00309

```

```

00310 VPRIVATE Vrc_Codes PBAMparm_parsePBCS(PBAMparm *thee, Vio *sock){
00311     const char* name = "pbc";
00312     char tok[VMAX_BUFSIZE];
00313     double tf;
00314     int td;
00315     if(Vio_scanf(sock, "%s", tok) == 0) {
00316         Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00317         return VRC_WARNING;
00318     }
00319
00320     if (sscanf(tok, "%d", &td) == 0) {
00321         Vnm_print(2, "parsePBAM: Read non-int (%s) while parsing pbc keyword!\n", tok);
00322         return VRC_FAILURE;
00323     } else{
00324         thee->setpbc = td;
00325     }
00326
00327     if (sscanf(tok, "%lf", &tf) == 0){
00328         Vnm_print(2, "Nosh: Read non-float (%s) while parsing %s keyword!\n", tok, name);
00329         return VRC_WARNING;
00330     }else{
00331         thee->pbcboxlen = tf;
00332     }
00333     return VRC_SUCCESS;
00334 }
00335
00336 VPRIVATE Vrc_Codes PBAMparm_parseUnits(PBAMparm *thee, Vio *sock){
00337     const char* name = "units";
00338     char tok[VMAX_BUFSIZE];
00339
00340     if(Vio_scanf(sock, "%s", tok) == 0) {
00341         Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00342         return VRC_WARNING;
00343     } else {
00344         strncpy(thee->units, tok, CHR_MAXLEN);
00345         thee->setunits=1;
00346     }
00347
00348     return VRC_SUCCESS;
00349 }
00350
00351 VPRIVATE Vrc_Codes PBAMparm_parseGridPts(PBAMparm *thee, Vio *sock){
00352     const char* name = "dime";
00353     char tok[VMAX_BUFSIZE];
00354     int td;
00355     if(Vio_scanf(sock, "%s", tok) == 0) {
00356         Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00357         return VRC_WARNING;
00358     }
00359
00360     if (sscanf(tok, "%d", &td) == 0){
00361         Vnm_print(2, "Nosh: Read non-integer (%s) while parsing %s keyword!\n", tok, name);
00362         return VRC_WARNING;
00363     }else{
00364         printf("Found a dime flag in parse: %d\n", td);
00365         thee->gridpt = td;
00366     }
00367     thee->setgridpt = 1;
00368     return VRC_SUCCESS;
00369 }
00370
00371 VPRIVATE Vrc_Codes PBAMparm_parse3Dmap(PBAMparm *thee, Vio *sock){
00372     const char* name = "3dmap";
00373     char tok[VMAX_BUFSIZE];
00374
00375     Vnm_print(2, "PBAM: 3dmap keyword has been deprecated! Please use in conjunction with the write
keyword.");
00376     return VRC_FAILURE;
00377
00378     /*
00379     if(Vio_scanf(sock, "%s", tok) == 0) {
00380         Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00381         return VRC_WARNING;
00382     } else {
00383         strncpy(thee->map3dname, tok, CHR_MAXLEN);
00384         thee->set3dmap=1;
00385     }
00386
00387     return VRC_SUCCESS;
00388     */
00389 }

```

```

00390
00391 VPRIVATE Vrc_Codes PBAMparm_parseGrid2D(PBAMparm *thee, Vio *sock){
00392     const char* name = "grid2d";
00393     char tok[VMAX_BUFSIZE];
00394     double tf;
00395
00396     if(Vio_scanf(sock, "%s", tok) == 0) {
00397         Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00398         return VRC_WARNING;
00399     } else {
00400         strncpy(thee->grid2Dname[thee->grid2Dct], tok, CHR_MAXLEN);
00401         thee->setgrid2Dname=1;
00402     }
00403
00404     if(Vio_scanf(sock, "%s", tok) == 0) {
00405         Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00406         return VRC_WARNING;
00407     } else {
00408         strncpy(thee->grid2Dax[thee->grid2Dct], tok, CHR_MAXLEN);
00409     }
00410
00411     if(Vio_scanf(sock, "%s", tok) == 0) {
00412         Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00413         return VRC_WARNING;
00414     }
00415
00416     if (sscanf(tok, "%lf", &tf) == 0){
00417         Vnm_print(2, "Nosh: Read non-float (%s) while parsing %s keyword!\n", tok, name);
00418         return VRC_WARNING;
00419     }else{
00420         thee->grid2Dloc[thee->grid2Dct] = tf;
00421         thee->grid2Dct = thee->grid2Dct+1;
00422     }
00423     return VRC_SUCCESS;
00424 }
00425
00426 VPRIVATE Vrc_Codes PBAMparm_parseDX(PBAMparm *thee, Vio *sock){
00427     Vnm_print(2, "PBAM's dx keyword is deprecated. Please use the write keyword!\n");
00428     return VRC_FAILURE;
00429     /*
00430     const char* name = "dx";
00431     char tok[VMAX_BUFSIZE];
00432
00433     if(Vio_scanf(sock, "%s", tok) == 0) {
00434         Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00435         return VRC_WARNING;
00436     } else {
00437         strncpy(thee->dxname, tok, CHR_MAXLEN);
00438         thee->setdxname=1;
00439     }
00440     return VRC_SUCCESS;
00441     */
00442 }
00443
00444 VPRIVATE Vrc_Codes PBAMparm_parseTermcombine(PBAMparm *thee, Vio *sock){
00445     const char* name = "termcombine";
00446     char tok[VMAX_BUFSIZE];
00447
00448     if(Vio_scanf(sock, "%s", tok) == 0) {
00449         Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00450         return VRC_WARNING;
00451     } else {
00452         strncpy(thee->termcombine, tok, CHR_MAXLEN);
00453         thee->settermcombine=1;
00454     }
00455     return VRC_SUCCESS;
00456 }
00457
00458 VPRIVATE Vrc_Codes PBAMparm_parseNtraj(PBAMparm *thee, Vio *sock){
00459     const char* name = "ntraj";
00460     char tok[VMAX_BUFSIZE];
00461     int td;
00462     if(Vio_scanf(sock, "%s", tok) == 0) {
00463         Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00464         return VRC_WARNING;
00465     }
00466
00467     if (sscanf(tok, "%d", &td) == 0){
00468         Vnm_print(2, "Nosh: Read non-integer (%s) while parsing %s keyword!\n", tok, name);
00469         return VRC_WARNING;
00470     }else{

```

```

00471     thee->ntraj = td;
00472 }
00473 thee->setntraj = 1;
00474 return VRC_SUCCESS;
00475 }
00476
00477 VPRIVATE Vrc_Codes PBAMparm_parseDiff(PBAMparm *thee, Vio *sock){
00478     const char* name = "diff";
00479     char tok[VMAX_BUFSIZE];
00480     int molind;
00481     double tf;
00482
00483     if(Vio_scanf(sock, "%s", tok) == 0) {
00484         Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00485         return VRC_WARNING;
00486     }
00487
00488     // // looking for index
00489     if (sscanf(tok, "%d", &molind) == 0){
00490         Vnm_print(2, "Nosh: Read non-int (%s) while parsing %s keyword!\n", tok, name);
00491         return VRC_WARNING;
00492     }
00493
00494     molind -= 1;
00495     // looking for move type = move, stat, rot
00496     if(Vio_scanf(sock, "%s", tok) == 0) {
00497         Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00498         return VRC_WARNING;
00499     } else {
00500         strncpy(thee->moveType[molind], tok, CHR_MAXLEN);
00501         thee->diffct += 1;
00502     }
00503
00504     if (strcmp(thee->moveType[molind], "move", 4) == 0)
00505     {
00506         if(Vio_scanf(sock, "%s", tok) == 0) {
00507             Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00508             return VRC_WARNING;
00509         }
00510         if (sscanf(tok, "%lf", &tf) == 0){
00511             Vnm_print(2, "Nosh: Read non-float (%s) while parsing %s keyword!\n", tok, name);
00512             return VRC_WARNING;
00513         }else{
00514             thee->transDiff[molind] = tf;
00515         }
00516
00517         // rot diffusion coeff
00518         if(Vio_scanf(sock, "%s", tok) == 0) {
00519             Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00520             return VRC_WARNING;
00521         }
00522         if (sscanf(tok, "%lf", &tf) == 0){
00523             Vnm_print(2, "Nosh: Read non-float (%s) while parsing %s keyword!\n", tok, name);
00524             return VRC_WARNING;
00525         }else{
00526             thee->rotDiff[molind] = tf;
00527         }
00528     } else if (strcmp(thee->moveType[molind], "rot", 3) == 0)
00529     {
00530         if(Vio_scanf(sock, "%s", tok) == 0) {
00531             Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00532             return VRC_WARNING;
00533         }
00534         if (sscanf(tok, "%lf", &tf) == 0){
00535             Vnm_print(2, "Nosh: Read non-float (%s) while parsing %s keyword!\n", tok, name);
00536             return VRC_WARNING;
00537         }else{
00538             thee->rotDiff[molind] = tf;
00539             thee->transDiff[molind] = 0.0;
00540         }
00541     } else{
00542         thee->transDiff[molind] = 0.0;
00543         thee->rotDiff[molind] = 0.0;
00544     }
00545
00546     return VRC_SUCCESS;
00547 }
00548
00549 VPRIVATE Vrc_Codes PBAMparm_parseTerm(PBAMparm *thee, Vio *sock){
00550     const char* name = "term";
00551     char tok[VMAX_BUFSIZE];

```

```

00552     double tf;
00553     int td;
00554
00555     // looking for term name
00556     if (Vio_scanf(sock, "%s", tok) == 0) {
00557         Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00558         return VRC_WARNING;
00559     } else {
00560         if (strcmp(tok, "position", 8) == 0) {
00561             return PBAMparm_parseTerm(thee, sock);
00562         } else {
00563             strncpy(thee->termnam[thee->termct], tok, CHR_MAXLEN);
00564         }
00565     }
00566
00567     if (strcmp(thee->termnam[thee->termct], "contact", 7) == 0)
00568     {
00569         if (Vio_scanf(sock, "%s", tok) == 0) {
00570             Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00571             return VRC_WARNING;
00572         } else {
00573             strncpy(thee->confil[thee->confilct], tok, CHR_MAXLEN);
00574         }
00575
00576         if (Vio_scanf(sock, "%s", tok) == 0) {
00577             Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00578             return VRC_WARNING;
00579         }
00580         if (sscanf(tok, "%lf", &tf) == 0) {
00581             Vnm_print(2, "NOsh: Read non-float (%s) while parsing %s keyword!\n", tok, name);
00582             return VRC_WARNING;
00583         } else {
00584             {
00585                 thee->termVal[thee->termct] = tf;
00586                 thee->termnu[thee->termct][0] = 0;
00587                 thee->confilct += 1;
00588             }
00589         } else if (strcmp(thee->termnam[thee->termct], "time", 4) == 0)
00590         {
00591             if (Vio_scanf(sock, "%s", tok) == 0) {
00592                 Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00593                 return VRC_WARNING;
00594             }
00595             if (sscanf(tok, "%lf", &tf) == 0) {
00596                 Vnm_print(2, "NOsh: Read non-float (%s) while parsing %s keyword!\n", tok, name);
00597                 return VRC_WARNING;
00598             } else {
00599                 thee->termVal[thee->termct] = tf;
00600                 thee->termnu[thee->termct][0] = 0;
00601             }
00602         } else //if (strcmp(thee->termnam[thee->termct], "position", 8) == 0)
00603         {
00604             if (Vio_scanf(sock, "%s", tok) == 0) {
00605                 Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00606                 return VRC_WARNING;
00607             }
00608             if (sscanf(tok, "%lf", &tf) == 0) {
00609                 Vnm_print(2, "NOsh: Read non-float (%s) while parsing %s keyword!\n", tok, name);
00610                 return VRC_WARNING;
00611             } else {
00612                 thee->termVal[thee->termct] = tf;
00613             }
00614
00615             if (Vio_scanf(sock, "%s", tok) == 0) {
00616                 Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00617                 return VRC_WARNING;
00618             }
00619             if (sscanf(tok, "%d", &td) == 0) {
00620                 Vnm_print(2, "NOsh: Read non-float (%s) while parsing %s keyword!\n", tok, name);
00621                 return VRC_WARNING;
00622             } else {
00623                 thee->termnu[thee->termct][0] = td-1;
00624             }
00625         }
00626
00627         thee->setterm = 1;
00628         thee->termct += 1;
00629         return VRC_SUCCESS;
00630     }
00631
00632 VPRIVATE Vrc_Codes PBAMparm_parseXYZ(PBAMparm *thee, Vio *sock){

```



```
00633     const char* name = "xyz";
00634     char tok[VMAX_BUFSIZE];
00635     int td, mol;
00636
00637     if (Vio_scanf(sock, "%s", tok) == 0) {
00638         Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00639         return VRC_WARNING;
00640     }
00641
00642     // // looking for index
00643     if (sscanf(tok, "%d", &td) == 0) {
00644         Vnm_print(2, "Nosh: Read non-int (%s) while parsing %s keyword!\n", tok, name);
00645         return VRC_WARNING;
00646     } else {
00647         printf("This is my mol in parseXYZ: %d", td);
00648         mol = td-1;
00649     }
00650
00651     // looking for move type = move, stat, rot
00652     if (Vio_scanf(sock, "%s", tok) == 0) {
00653         Vnm_print(2, "parsePBAM: ran out of tokens on %s!\n", name);
00654         return VRC_WARNING;
00655     } else {
00656         strncpy(thee->xyzfil[mol][thee->xyzct[mol]], tok, CHR_MAXLEN);
00657         thee->xyzct[mol] += 1;
00658     }
00659     return VRC_SUCCESS;
00660 }
00661
00662 VPUBLIC Vrc_Codes PBAMparm_parseToken(PBAMparm *thee, char tok[VMAX_BUFSIZE],
00663 Vio *sock) {
00664
00665     if (thee == VNULL) {
00666         Vnm_print(2, "parsePBAM: got NULL thee!\n");
00667         return VRC_WARNING;
00668     }
00669     if (sock == VNULL) {
00670         Vnm_print(2, "parsePBAM: got NULL socket!\n");
00671         return VRC_WARNING;
00672     }
00673
00674     Vnm_print(0, "PBAMparm_parseToken: trying %s...\n", tok);
00675
00676     // General terms to parse
00677     if (Vstring_strcasecmp(tok, "salt") == 0) {
00678         return PBAMparm_parseSalt(thee, sock);
00679     } else if (Vstring_strcasecmp(tok, "runtype") == 0) {
00680         return PBAMparm_parseRunType(thee, sock);
00681     } else if (Vstring_strcasecmp(tok, "runname") == 0) {
00682         return PBAMparm_parseRunName(thee, sock);
00683     } else if (Vstring_strcasecmp(tok, "randorient") == 0) {
00684         return PBAMparm_parseRandorient(thee, sock);
00685     } else if (Vstring_strcasecmp(tok, "pbc") == 0) {
00686         return PBAMparm_parsePBCS(thee, sock);
00687     } else if (Vstring_strcasecmp(tok, "units") == 0) {
00688         return PBAMparm_parseUnits(thee, sock);
00689     }
00690
00691     // Electrostatic parsing
00692     else if (Vstring_strcasecmp(tok, "dime") == 0) {
00693         return PBAMparm_parseGridPts(thee, sock);
00694     } else if (Vstring_strcasecmp(tok, "3dmap") == 0) {
00695         return PBAMparm_parse3Dmap(thee, sock);
00696     } else if (Vstring_strcasecmp(tok, "grid2d") == 0) {
00697         return PBAMparm_parseGrid2D(thee, sock);
00698     } else if (Vstring_strcasecmp(tok, "dx") == 0) {
00699         return PBAMparm_parseDX(thee, sock);
00700     }
00701
00702     // Dynamics parsing
00703     else if (Vstring_strcasecmp(tok, "ntraj") == 0) {
00704         return PBAMparm_parseNtraj(thee, sock);
00705     } else if (Vstring_strcasecmp(tok, "termcombine") == 0) {
00706         return PBAMparm_parseTermcombine(thee, sock);
00707     } else if (Vstring_strcasecmp(tok, "diff") == 0) {
00708         return PBAMparm_parseDiff(thee, sock);
00709     } else if (Vstring_strcasecmp(tok, "term") == 0) {
00710         return PBAMparm_parseTerm(thee, sock);
00711     } else if (Vstring_strcasecmp(tok, "xyz") == 0) {
00712         return PBAMparm_parseXYZ(thee, sock);
00713     }
}
```

```

00714
00715
00716     else
00717         return 0;
00718
00719     /*else {
00720         Vnm_print(2, "parsePBAM: Unrecognized keyword (%s)!\n", tok);
00721         return VRC_WARNING;
00722     }
00723     return VRC_FAILURE;
00724 */
00725 }

```

9.40 src/generic/pbamparm.h File Reference

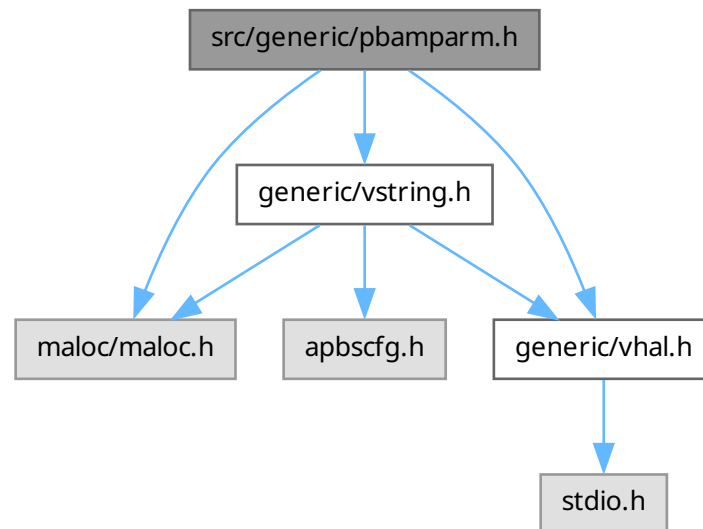
Contains declarations for class PBAMparm.

```
#include "maloc/maloc.h"
```

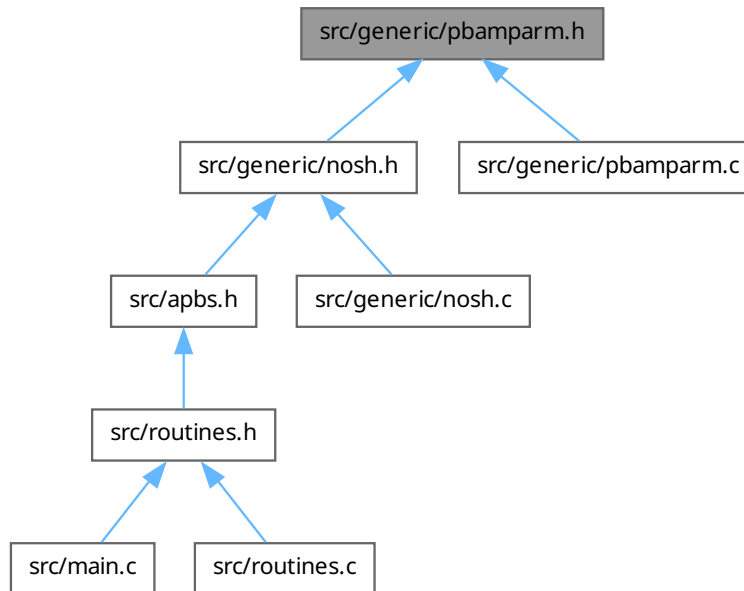
```
#include "generic/vhal.h"
```

```
#include "generic/vstring.h"
```

Include dependency graph for pbamparm.h:



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [sPBAMparm](#)
Parameter structure for PBAM-specific variables from input files.

Macros

- #define [CHR_MAXLEN](#) 1000
Number of things that can be written out in a single calculation.
- #define [PBAMPARM_MAXWRITE](#) 15
- #define [PBAMPARM_MAXMOL](#) 150

Typedefs

- typedef enum [ePBAMparm_CalcType](#) [PBAMparm_CalcType](#)
Declare PBAMparm_CalcType type.
- typedef struct [sPBAMparm](#) [PBAMparm](#)
Parameter structure for PBAM-specific variables from input files.

Enumerations

- enum [ePBAMparm_CalcType](#) { [PBAMCT_AUTO](#) =1 }
- Calculation type.*

Functions

- VEXTERNC PBAMparm * PBAMparm_ctor (PBAMparm_CalcType type)
Construct PBAMparm object.
- VEXTERNC Vrc_Codes PBAMparm_ctor2 (PBAMparm *thee, PBAMparm_CalcType type)
FORTTRAN stub to construct PBAMparm object ?????????!!!!!!
- VEXTERNC void PBAMparm_dtor (PBAMparm **thee)
Object destructor.
- VEXTERNC void PBAMparm_dtor2 (PBAMparm *thee)
FORTTRAN stub for object destructor ?????????!!!!!!
- VEXTERNC Vrc_Codes PBAMparm_check (PBAMparm *thee)
Consistency check for parameter values stored in object.
- VEXTERNC Vrc_Codes PBAMparm_parseToken (PBAMparm *thee, char tok[VMAX_BUFSIZE], Vio *sock)
Parse an MG keyword from an input file.
- VEXTERNC void PBAMparm_copy (PBAMparm *thee, PBAMparm *parm)
copy PBAMparm object into thee.
- VPRIVATE Vrc_Codes PBAMparm_parseSalt (PBAMparm *thee, Vio *sock)
Find salt conc and save it as a structure variable.
- VPRIVATE Vrc_Codes PBAMparm_parseRunType (PBAMparm *thee, Vio *sock)
Find runType and save it as a structure variable.
- VPRIVATE Vrc_Codes PBAMparm_parseRunName (PBAMparm *thee, Vio *sock)
Find runName and save it as a structure variable.
- VPRIVATE Vrc_Codes PBAMparm_parseRandorient (PBAMparm *thee, Vio *sock)
Find randomorientation flag and save it as a boolean.
- VPRIVATE Vrc_Codes PBAMparm_parsePBCS (PBAMparm *thee, Vio *sock)
Find PBC flag and save the type and the boxlength.
- VPRIVATE Vrc_Codes PBAMparm_parseUnits (PBAMparm *thee, Vio *sock)
Find units flag and save units.
- VPRIVATE Vrc_Codes PBAMparm_parse3Dmap (PBAMparm *thee, Vio *sock)
Find 3D map filename and save it.
- VPRIVATE Vrc_Codes PBAMparm_parseGrid2D (PBAMparm *thee, Vio *sock)
Find 2D grid filename and save it.
- VPRIVATE Vrc_Codes PBAMparm_parseDX (PBAMparm *thee, Vio *sock)
Find DX filename and save it.
- VPRIVATE Vrc_Codes PBAMparm_parseGridPts (PBAMparm *thee, Vio *sock)
Find Grid points and save them.
- VPRIVATE Vrc_Codes PBAMparm_parseTermcombine (PBAMparm *thee, Vio *sock)
Find Termination logic and save it.
- VPRIVATE Vrc_Codes PBAMparm_parseDiff (PBAMparm *thee, Vio *sock)
Find diffusion coeffs for each molecule and save them.
- VPRIVATE Vrc_Codes PBAMparm_parseXYZ (PBAMparm *thee, Vio *sock)
Find xyz files for each molecule for each traj and save them.

9.40.1 Detailed Description

Contains declarations for class PBAMparm.

Version

\$Id\$

Author

Lisa Felberg

Attention

```
*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
* Nathan A. Baker (nathan.baker@pnnl.gov)
* Pacific Northwest National Laboratory
*
* Additional contributing authors listed in the code documentation.
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* THE POSSIBILITY OF SUCH DAMAGE.
*
*
```

Definition in file [pbamparm.h](#).

9.40.2 Macro Definition Documentation

9.40.2.1 PBAMPARM_MAXMOL

```
#define PBAMPARM_MAXMOL 150
```

Definition at line 78 of file [pbamparm.h](#).

9.40.2.2 PBAMPARM_MAXWRITE

```
#define PBAMPARM_MAXWRITE 15
```

Definition at line 77 of file [pbamparm.h](#).

9.41 pbamparm.h

[Go to the documentation of this file.](#)

```
00001
00064 #ifndef _PBAMPARM_H_
00065 #define _PBAMPARM_H_
00066
00067 /* Generic header files */
00068 #include "malloc/malloc.h"
00069
00070 #include "generic/vhal.h"
00071 #include "generic/vstring.h"
00072
00076 #define CHR_MAXLEN 1000
00077 #define PBAMPARM_MAXWRITE 15
00078 #define PBAMPARM_MAXMOL 150
00079
00084 enum ePBAMParm_CalcType {
00085     //other methods disabled for now only auto currently implemented.
00086     //PBAMCT_MANUAL=0,    /**< PBAM-manual */
00087     PBAMCT_AUTO=1,
00088     //PBAMCT_NONE=2 /**< not defined */
00089 };
00090
00095 typedef enum ePBAMParm_CalcType PBAMParm_CalcType;
00096
00105 typedef struct sPBAMParm {
00106
00107     PBAMParm_CalcType type;
00108     int parsed;
00110     /* *** GENERIC PARAMETERS *** */
00111     double salt;
00112     int setsalt;
00113
00114     // This is the type of run you want
00115     char runtime[CHR_MAXLEN];
00116     int setruntime;
00117
00118     // This is the name for output files
00119     char runname[CHR_MAXLEN];
00120     int setrunname;
00121
00122     // For setting random orientation of molecules
00123     int setrandorient;
00124
00125     // For periodic boundary conditions
00126     double pbcbboxlen;
00127     int setpbcs;
00128
00129     // This is units of the calculation
00130     char units[CHR_MAXLEN];
00131     int setunits;
00132
00133     //
00134     // ELECTROSTATICS
00135     //
00136     // For the grid, store gridpt
00137     int gridpt;
00138     int setgridpt;
00139
00140     // For 3d map printing
00141     char map3dname[CHR_MAXLEN];
00142     int set3dmap;
00143
00144     // For 2D
00145     char grid2Dname[PBAMPARM_MAXWRITE][CHR_MAXLEN];
00146     char grid2Dax[PBAMPARM_MAXWRITE][CHR_MAXLEN];
00147     double grid2Dloc[PBAMPARM_MAXWRITE];
00148     int grid2Dct;
```

```

00149     int setgrid2Dname;
00150
00151     // For dx
00152     char dxname[CHR_MAXLEN];
00153     int setdxname;
00154
00155     //
00156     // DYNAMICS
00157     //
00158     int ntraj;
00159     int setntraj;
00160
00161     char termcombine[CHR_MAXLEN];
00162     int settermcombine;
00163
00164     int diffct;
00165     char moveType[PBAMPARM_MAXMOL][CHR_MAXLEN];
00166     double transDiff[PBAMPARM_MAXMOL];
00167     double rotDiff[PBAMPARM_MAXMOL];
00168
00169     int termct;
00170     int setterm;
00171
00172     char termnam[PBAMPARM_MAXWRITE][CHR_MAXLEN];
00173     int termnu[PBAMPARM_MAXWRITE][1];
00174     double termVal[PBAMPARM_MAXWRITE];
00175     char confil[PBAMPARM_MAXWRITE][CHR_MAXLEN];
00176     double conpad[PBAMPARM_MAXWRITE];
00177     int confilct;
00178
00179     int setxyz;
00180     int xyzct[PBAMPARM_MAXMOL];
00181     char xyzfil[PBAMPARM_MAXMOL][PBAMPARM_MAXWRITE][CHR_MAXLEN];
00182
00183 } PBAMParm;
00184
00191 VEXTERNC PBAMParm* PBAMParm_ctor(PBAMParm_CalcType type);
00192
00200 VEXTERNC Vrc_Codes PBAMParm_ctor2(PBAMParm *thee, PBAMParm_CalcType type);
00201
00207 VEXTERNC void PBAMParm_dtor(PBAMParm **thee);
00208
00214 VEXTERNC void PBAMParm_dtor2(PBAMParm *thee);
00215
00222 VEXTERNC Vrc_Codes PBAMParm_check(PBAMParm *thee);
00223
00233 VEXTERNC Vrc_Codes PBAMParm_parseToken(PBAMParm *thee, char tok[VMAX_BUFSIZE],
00234                                         Vio *sock);
00242 VEXTERNC void PBAMParm_copy(PBAMParm *thee, PBAMParm *parm);
00243
00251 VPRIVATE Vrc_Codes PBAMParm_parseSalt(PBAMParm *thee, Vio *sock);
00252
00260 VPRIVATE Vrc_Codes PBAMParm_parseRunType(PBAMParm *thee, Vio *sock);
00261
00269 VPRIVATE Vrc_Codes PBAMParm_parseRunName(PBAMParm *thee, Vio *sock);
00270
00278 VPRIVATE Vrc_Codes PBAMParm_parseRandorient(PBAMParm *thee, Vio *sock);
00279
00287 VPRIVATE Vrc_Codes PBAMParm_parsePBCS(PBAMParm *thee, Vio *sock);
00288
00296 VPRIVATE Vrc_Codes PBAMParm_parseUnits(PBAMParm *thee, Vio *sock);
00297
00305 VPRIVATE Vrc_Codes PBAMParm_parse3Dmap(PBAMParm *thee, Vio *sock);
00306
00314 VPRIVATE Vrc_Codes PBAMParm_parseGrid2D(PBAMParm *thee, Vio *sock);
00315
00323 VPRIVATE Vrc_Codes PBAMParm_parseDX(PBAMParm *thee, Vio *sock);
00324
00332 VPRIVATE Vrc_Codes PBAMParm_parseGridPts(PBAMParm *thee, Vio *sock);
00333
00341 VPRIVATE Vrc_Codes PBAMParm_parseTermcombine(PBAMParm *thee, Vio *sock);
00342
00350 VPRIVATE Vrc_Codes PBAMParm_parseDiff(PBAMParm *thee, Vio *sock);
00351
00359 VPRIVATE Vrc_Codes PBAMParm_parseXYZ(PBAMParm *thee, Vio *sock);
00360
00361
00362
00363
00364 #endif
00365

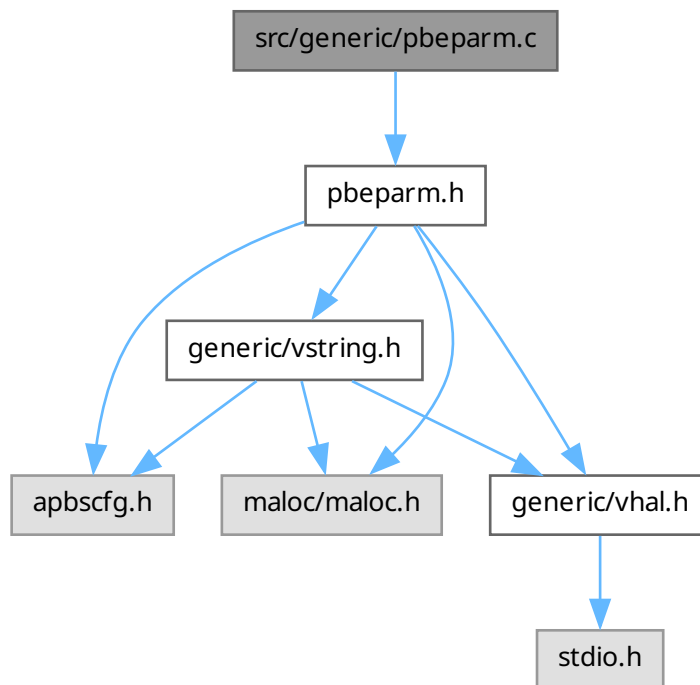
```

9.42 src/generic/pbeparm.c File Reference

Class PBEparm methods.

```
#include "pbeparm.h"
```

Include dependency graph for pbeparm.c:



Functions

- VPUBLIC double [PBEparm_getIonCharge](#) (PBEparm *thee, int i)
Get charge (e) of specified ion species.
- VPUBLIC double [PBEparm_getIonConc](#) (PBEparm *thee, int i)
Get concentration (M) of specified ion species.
- VPUBLIC double [PBEparm_getIonRadius](#) (PBEparm *thee, int i)
Get radius (Å) of specified ion species.
- VPUBLIC double [PBEparm_getzmem](#) (PBEparm *thee)
- VPUBLIC double [PBEparm_getLmem](#) (PBEparm *thee)
- VPUBLIC double [PBEparm_getmembraneDiel](#) (PBEparm *thee)
- VPUBLIC double [PBEparm_getmemv](#) (PBEparm *thee)
- VPUBLIC PBEparm * [PBEparm_ctor](#) ()
Construct PBEparm object.
- VPUBLIC int [PBEparm_ctor2](#) (PBEparm *thee)
FORTTRAN stub to construct PBEparm object.
- VPUBLIC void [PBEparm_dtor](#) (PBEparm **thee)

Object destructor.

- VPUBLIC void [PBEParm_dtor2](#) (PBEParm *thee)

FORTTRAN stub for object destructor.

- VPUBLIC int [PBEParm_check](#) (PBEParm *thee)

Consistency check for parameter values stored in object.

- VPUBLIC void [PBEParm_copy](#) (PBEParm *thee, PBEParm *parm)

Copy PBEParm object into thee.

- VPRIVATE int [PBEParm_parseLPBE](#) (PBEParm *thee, Vio *sock)
- VPRIVATE int [PBEParm_parseNPBE](#) (PBEParm *thee, Vio *sock)
- VPRIVATE int [PBEParm_parseMOL](#) (PBEParm *thee, Vio *sock)
- VPRIVATE int [PBEParm_parseLRPBE](#) (PBEParm *thee, Vio *sock)
- VPRIVATE int [PBEParm_parseNRPBE](#) (PBEParm *thee, Vio *sock)
- VPRIVATE int [PBEParm_parseSMPBE](#) (PBEParm *thee, Vio *sock)
- VPRIVATE int [PBEParm_parseBCFL](#) (PBEParm *thee, Vio *sock)
- VPRIVATE int [PBEParm_parseION](#) (PBEParm *thee, Vio *sock)
- VPRIVATE int [PBEParm_parsePDIE](#) (PBEParm *thee, Vio *sock)
- VPRIVATE int [PBEParm_parseSDENS](#) (PBEParm *thee, Vio *sock)
- VPRIVATE int [PBEParm_parseSDIE](#) (PBEParm *thee, Vio *sock)
- VPRIVATE int [PBEParm_parseSRFM](#) (PBEParm *thee, Vio *sock)
- VPRIVATE int [PBEParm_parseSRAD](#) (PBEParm *thee, Vio *sock)
- VPRIVATE int [PBEParm_parseSWIN](#) (PBEParm *thee, Vio *sock)
- VPRIVATE int [PBEParm_parseTEMP](#) (PBEParm *thee, Vio *sock)
- VPRIVATE int [PBEParm_parseUSEMAP](#) (PBEParm *thee, Vio *sock)
- VPRIVATE int [PBEParm_parseCALCENERGY](#) (PBEParm *thee, Vio *sock)
- VPRIVATE int [PBEParm_parseCALCFORCE](#) (PBEParm *thee, Vio *sock)
- VPRIVATE int [PBEParm_parseZMEM](#) (PBEParm *thee, Vio *sock)
- VPRIVATE int [PBEParm_parseLMEM](#) (PBEParm *thee, Vio *sock)
- VPRIVATE int [PBEParm_parseMDIE](#) (PBEParm *thee, Vio *sock)
- VPRIVATE int [PBEParm_parseMEMV](#) (PBEParm *thee, Vio *sock)
- VPRIVATE int [PBEParm_parseWRITE](#) (PBEParm *thee, Vio *sock)
- VPRIVATE int [PBEParm_parseWRITEMAT](#) (PBEParm *thee, Vio *sock)
- VPUBLIC int [PBEParm_parseToken](#) (PBEParm *thee, char tok[VMAX_BUFSIZE], Vio *sock)

Parse a keyword from an input file.

9.42.1 Detailed Description

Class PBEParm methods.

Author

Nathan Baker

Version

\$Id\$

Attention

```

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*
*

```

Definition in file [pbeparm.c](#).

9.42.2 Function Documentation**9.42.2.1 PBEparm_getLmem()**

```

VPUBLIC double PBEparm_getLmem (
    PBEparm * thee )

```

Definition at line 91 of file [pbeparm.c](#).

9.42.2.2 PBEparm_getmembraneDiel()

```

VPUBLIC double PBEparm_getmembraneDiel (
    PBEparm * thee )

```

Definition at line 95 of file [pbeparm.c](#).

9.42.2.3 PBEparm_getmemv()

```
VPUBLIC double PBEparm_getmemv (  
    PBEparm * thee )
```

Definition at line 99 of file [pbeparm.c](#).

9.42.2.4 PBEparm_getzmem()

```
VPUBLIC double PBEparm_getzmem (  
    PBEparm * thee )
```

Definition at line 87 of file [pbeparm.c](#).

9.42.2.5 PBEparm_parseBCFL()

```
VPRIVATE int PBEparm_parseBCFL (  
    PBEparm * thee,  
    Vio * sock )
```

Definition at line 474 of file [pbeparm.c](#).

9.42.2.6 PBEparm_parseCALCENERGY()

```
VPRIVATE int PBEparm_parseCALCENERGY (  
    PBEparm * thee,  
    Vio * sock )
```

Definition at line 895 of file [pbeparm.c](#).

9.42.2.7 PBEparm_parseCALCFORCE()

```
VPRIVATE int PBEparm_parseCALCFORCE (  
    PBEparm * thee,  
    Vio * sock )
```

Definition at line 948 of file [pbeparm.c](#).

9.42.2.8 PBEparm_parseION()

```
VPRIVATE int PBEparm_parseION (  
    PBEparm * thee,  
    Vio * sock )
```

Definition at line 555 of file [pbeparm.c](#).

9.42.2.9 PBEparm_parseLMEM()

```
VPRIVATE int PBEparm_parseLMEM (  
    PBEparm * thee,  
    Vio * sock )
```

Definition at line 1025 of file [pbeparm.c](#).

9.42.2.10 PBEparm_parseLPBE()

```
VPRIVATE int PBEparm_parseLPBE (  
    PBEparm * thee,  
    Vio * sock )
```

Definition at line 368 of file [pbeparm.c](#).

9.42.2.11 PBEparm_parseLRPBE()

```
VPRIVATE int PBEparm_parseLRPBE (  
    PBEparm * thee,  
    Vio * sock )
```

Definition at line 401 of file [pbeparm.c](#).

9.42.2.12 PBEparm_parseMDIE()

```
VPRIVATE int PBEparm_parseMDIE (  
    PBEparm * thee,  
    Vio * sock )
```

Definition at line 1044 of file [pbeparm.c](#).

9.42.2.13 PBEparm_parseMEMV()

```
VPRIVATE int PBEparm_parseMEMV (  
    PBEparm * thee,  
    Vio * sock )
```

Definition at line 1063 of file [pbeparm.c](#).

9.42.2.14 PBEparm_parseMOL()

```
VPRIVATE int PBEparm_parseMOL (  
    PBEparm * thee,  
    Vio * sock )
```

Definition at line 382 of file [pbeparm.c](#).

9.42.2.15 PBEparm_parseNPBE()

```
VPRIVATE int PBEparm_parseNPBE (  
    PBEparm * thee,  
    Vio * sock )
```

Definition at line 375 of file [pbeparm.c](#).

9.42.2.16 PBEparm_parseNRPBE()

```
VPRIVATE int PBEparm_parseNRPBE (  
    PBEparm * thee,  
    Vio * sock )
```

Definition at line 408 of file [pbeparm.c](#).

9.42.2.17 PBEparm_parsePDIE()

```
VPRIVATE int PBEparm_parsePDIE (  
    PBEparm * thee,  
    Vio * sock )
```

Definition at line 652 of file [pbeparm.c](#).

9.42.2.18 PBEparm_parseSDENS()

```
VPRIVATE int PBEparm_parseSDENS (  
    PBEparm * thee,  
    Vio * sock )
```

Definition at line 671 of file [pbeparm.c](#).

9.42.2.19 PBEparm_parseSDIE()

```
VPRIVATE int PBEparm_parseSDIE (  
    PBEparm * thee,  
    Vio * sock )
```

Definition at line 690 of file [pbeparm.c](#).

9.42.2.20 PBEparm_parseSMPBE()

```
VPRIVATE int PBEparm_parseSMPBE (  
    PBEparm * thee,  
    Vio * sock )
```

Definition at line 415 of file [pbeparm.c](#).

9.42.2.21 PBEparm_parseSRAD()

```
VPRIVATE int PBEparm_parseSRAD (  
    PBEparm * thee,  
    Vio * sock )
```

Definition at line 780 of file [pbeparm.c](#).

9.42.2.22 PBEparm_parseSRFM()

```
VPRIVATE int PBEparm_parseSRFM (  
    PBEparm * thee,  
    Vio * sock )
```

Definition at line 709 of file [pbeparm.c](#).

9.42.2.23 PBEparm_parseSWIN()

```
VPRIVATE int PBEparm_parseSWIN (  
    PBEparm * thee,  
    Vio * sock )
```

Definition at line 799 of file [pbeparm.c](#).

9.42.2.24 PBEparm_parseTEMP()

```
VPRIVATE int PBEparm_parseTEMP (  
    PBEparm * thee,  
    Vio * sock )
```

Definition at line 818 of file [pbeparm.c](#).

9.42.2.25 PBEparm_parseUSEMAP()

```
VPRIVATE int PBEparm_parseUSEMAP (  
    PBEparm * thee,  
    Vio * sock )
```

Definition at line 837 of file [pbeparm.c](#).

9.42.2.26 PBEparm_parseWRITE()

```
VPRIVATE int PBEparm_parseWRITE (  
    PBEparm * thee,  
    Vio * sock )
```

Definition at line 1084 of file [pbeparm.c](#).

9.42.2.27 PBEparm_parseWRITEMAT()

```
VPRIVATE int PBEparm_parseWRITEMAT (
    PBEparm * thee,
    Vio * sock )
```

Definition at line 1178 of file [pbeparm.c](#).

9.42.2.28 PBEparm_parseZMEM()

```
VPRIVATE int PBEparm_parseZMEM (
    PBEparm * thee,
    Vio * sock )
```

Definition at line 1005 of file [pbeparm.c](#).

9.43 pbeparm.c

[Go to the documentation of this file.](#)

```
00001
00057 #include "pbeparm.h"
00058
00059 VEMBED(rcsid="$Id$")
00060
00061 #if !defined(VINLINE_MGPARM)
00062
00063 #endif /* if !defined(VINLINE_MGPARM) */
00064
00065 VPUBLIC double PBEparm_getIonCharge(PBEparm *thee, int i) {
00066     VASSERT(thee != VNULL);
00067     VASSERT(i < thee->nion);
00068     return thee->ionq[i];
00069 }
00070
00071 VPUBLIC double PBEparm_getIonConc(PBEparm *thee, int i) {
00072     VASSERT(thee != VNULL);
00073     VASSERT(i < thee->nion);
00074     return thee->ionc[i];
00075 }
00076
00077 VPUBLIC double PBEparm_getIonRadius(PBEparm *thee, int i) {
00078     VASSERT(thee != VNULL);
00079     VASSERT(i < thee->nion);
00080     return thee->ionr[i];
00081 }
00082
00083 /*-----*/
00084 /* Added by Michael Grabe */
00085 /*-----*/
00086
00087 VPUBLIC double PBEparm_getzmem(PBEparm *thee) {
00088     VASSERT(thee != VNULL);
00089     return thee->zmem;
00090 }
00091 VPUBLIC double PBEparm_getLmem(PBEparm *thee) {
00092     VASSERT(thee != VNULL);
00093     return thee->Lmem;
00094 }
00095 VPUBLIC double PBEparm_getmembraneDiel(PBEparm *thee) {
00096     VASSERT(thee != VNULL);
00097     return thee->mDie;
00098 }
00099 VPUBLIC double PBEparm_getmemv(PBEparm *thee) {
00100     VASSERT(thee != VNULL);
00101     return thee->memv;
00102 }
00103
00104 VPUBLIC PBEparm* PBEparm_ctor() {
00105
00106     /* Set up the structure */
00107     PBEparm *thee = VNULL;
00108     thee = (PBEparm*)Vmem_malloc(VNULL, 1, sizeof(PBEparm));
00109     VASSERT( thee != VNULL);
00110     VASSERT( PBEparm_ctor2(thee) );
00111 }
```

```

00112     return thee;
00113 }
00114
00115 VPUBLIC int PBEparm_ctor2(PBEparm *thee) {
00116     int i;
00117     if (thee == VNULL) return 0;
00118     thee->parsed = 0;
00119     thee->setmolid = 0;
00120     thee->setpbetype = 0;
00121     thee->setbcfl = 0;
00122     thee->setnion = 0;
00123     for (i=0; i<MAXION; i++){
00124         thee->setion[i] = 0;
00125         thee->ionq[i] = 0.0;
00126         thee->ionc[i] = 0.0;
00127         thee->ionr[i] = 0.0;
00128     }
00129     thee->setpdie = 0;
00130     thee->setsdie = 0;
00131     thee->setsrfm = 0;
00132     thee->setsrad = 0;
00133     thee->setswin = 0;
00134     thee->settemp = 0;
00135     thee->setcalcenergy = 0;
00136     thee->setcalcforce = 0;
00137     thee->setsdens = 0;
00138     thee->numwrite = 0;
00139     thee->setwritemat = 0;
00140     thee->nion = 0;
00141     thee->sdens = 0;
00142     thee->swin = 0;
00143     thee->srad = 1.4;
00144     thee->useDielMap = 0;
00145     thee->useKappaMap = 0;
00146     thee->usePotMap = 0;
00147     thee->useChargeMap = 0;
00148
00149     /*-----*/
00150     /* Added by Michael Grabe */
00151     /*-----*/
00152
00153     thee->setzmem = 0;
00154     thee->setlmem = 0;
00155     thee->setmdie = 0;
00156     thee->setmemv = 0;
00157
00158     /*-----*/
00159
00160     thee->smsize = 0.0;
00161     thee->smvolume = 0.0;
00162
00163     thee->setsmsize = 0;
00164     thee->setsmvolume = 0;
00165
00166     return 1;
00167 }
00168
00169 VPUBLIC void PBEparm_dtor(PBEparm **thee) {
00170     if ((*thee) != VNULL) {
00171         PBEparm_dtor2(*thee);
00172         Vmem_free(VNULL, 1, sizeof(PBEparm), (void **)thee);
00173         (*thee) = VNULL;
00174     }
00175 }
00176
00177 VPUBLIC void PBEparm_dtor2(PBEparm *thee) { ; }
00178
00179 VPUBLIC int PBEparm_check(PBEparm *thee) {
00180     int i;
00181
00182     /* Check to see if we were even filled... */
00183     if (!thee->parsed) {
00184         Vnm_print(2, "PBEparm_check: not filled!\n");
00185         return 0;
00186     }
00187 }
00188
00189

```

```

00193     if (!thee->setmolid) {
00194         Vnm_print(2, "PBEparm_check:  MOL not set!\n");
00195         return 0;
00196     }
00197     if (!thee->setpbetype) {
00198         Vnm_print(2, "PBEparm_check:  LPBE/NPBE/LRPBE/NRPBE/SMPBE not set!\n");
00199         return 0;
00200     }
00201     if (!thee->setbcfl) {
00202         Vnm_print(2, "PBEparm_check:  BCFL not set!\n");
00203         return 0;
00204     }
00205     if (!thee->setnion) {
00206         thee->setnion = 1;
00207         thee->nion = 0;
00208     }
00209     for (i=0; i<thee->nion; i++) {
00210         if (!thee->setion[i]) {
00211             Vnm_print(2, "PBEparm_check:  ION #%d not set!\n",i);
00212             return 0;
00213         }
00214     }
00215     if (!thee->setpdie) {
00216         Vnm_print(2, "PBEparm_check:  PDIE not set!\n");
00217         return 0;
00218     }
00219     if (((thee->srfm==VSM_MOL) || (thee->srfm==VSM_MOLSMOOTH)) \
00220         && (!thee->setsdens) && (thee->srad > VSMALL)) {
00221         Vnm_print(2, "PBEparm_check:  SDENS not set!\n");
00222         return 0;
00223     }
00224     if (!thee->setsdie) {
00225         Vnm_print(2, "PBEparm_check:  SDIE not set!\n");
00226         return 0;
00227     }
00228     if (!thee->setsrfm) {
00229         Vnm_print(2, "PBEparm_check:  SRFM not set!\n");
00230         return 0;
00231     }
00232     if (((thee->srfm==VSM_MOL) || (thee->srfm==VSM_MOLSMOOTH)) \
00233         && (!thee->setsrad)) {
00234         Vnm_print(2, "PBEparm_check:  SRAD not set!\n");
00235         return 0;
00236     }
00237     if ((thee->srfm==VSM_SPLINE) && (!thee->setswin)) {
00238         Vnm_print(2, "PBEparm_check:  SWIN not set!\n");
00239         return 0;
00240     }
00241     if ((thee->srfm==VSM_SPLINE3) && (!thee->setswin)) {
00242         Vnm_print(2, "PBEparm_check:  SWIN not set!\n");
00243         return 0;
00244     }
00245     if ((thee->srfm==VSM_SPLINE4) && (!thee->setswin)) {
00246         Vnm_print(2, "PBEparm_check:  SWIN not set!\n");
00247         return 0;
00248     }
00249     if (!thee->settemp) {
00250         Vnm_print(2, "PBEparm_check:  TEMP not set!\n");
00251         return 0;
00252     }
00253     if (!thee->setcalcenergy) thee->calcenergy = PCE_NO;
00254     if (!thee->setcalcforce) thee->calcforce = PCF_NO;
00255     if (!thee->setwritemat) thee->writemat = 0;
00256
00257     /*-----*/
00258     /* Added by Michael Grabe */
00259     /*-----*/
00260
00261     if ((!thee->setzmem) && (thee->bcfl == 3)){
00262         Vnm_print(2, "PBEparm_check:  ZMEM not set!\n");
00263         return 0;
00264     }
00265     if ((!thee->setlmem) && (thee->bcfl == 3)){
00266         Vnm_print(2, "PBEparm_check:  LMEM not set!\n");
00267         return 0;
00268     }
00269     if ((!thee->setmdie) && (thee->bcfl == 3)){
00270         Vnm_print(2, "PBEparm_check:  MDIE not set!\n");
00271         return 0;
00272     }
00273     if ((!thee->setmemv) && (thee->bcfl == 3)){

```



```

00274         Vnm_print(2, "PBeparm_check: MEMV not set!\n");
00275         return 0;
00276     }
00277
00278     /*-----*/
00279
00280     return 1;
00281 }
00282
00283 VPUBLIC void PBeparm_copy(PBeparm *thee, PBeparm *parm) {
00284
00285     int i, j;
00286
00287     VASSERT(thee != VNULL);
00288     VASSERT(parm != VNULL);
00289
00290     thee->molid = parm->molid;
00291     thee->setmolid = parm->setmolid;
00292     thee->useDielMap = parm->useDielMap;
00293     thee->dielMapID = parm->dielMapID;
00294     thee->useKappaMap = parm->useKappaMap;
00295     thee->kappaMapID = parm->kappaMapID;
00296     thee->usePotMap = parm->usePotMap;
00297     thee->potMapID = parm->potMapID;
00298     thee->useChargeMap = parm->useChargeMap;
00299     thee->chargeMapID = parm->chargeMapID;
00300     thee->pbetype = parm->pbetype;
00301     thee->setpbetype = parm->setpbetype;
00302     thee->bcfl = parm->bcfl;
00303     thee->setbcfl = parm->setbcfl;
00304     thee->nion = parm->nion;
00305     thee->setnion = parm->setnion;
00306     for (i=0; i<MAXION; i++) {
00307         thee->ionq[i] = parm->ionq[i];
00308         thee->ionc[i] = parm->ionc[i];
00309         thee->ionr[i] = parm->ionr[i];
00310         thee->setion[i] = parm->setion[i];
00311     };
00312     thee->pdie = parm->pdie;
00313     thee->setpdie = parm->setpdie;
00314     thee->sdens = parm->sdens;
00315     thee->setsdens = parm->setsdens;
00316     thee->sdiel = parm->sdiel;
00317     thee->setsdiel = parm->setsdiel;
00318     thee->srfm = parm->srfm;
00319     thee->setsrfm = parm->setsrfm;
00320     thee->srad = parm->srad;
00321     thee->setsrad = parm->setsrad;
00322     thee->swin = parm->swin;
00323     thee->setswin = parm->setswin;
00324     thee->temp = parm->temp;
00325     thee->settemp = parm->settemp;
00326     thee->calcenergy = parm->calcenergy;
00327     thee->setcalcenergy = parm->setcalcenergy;
00328     thee->calcforce = parm->calcforce;
00329     thee->setcalcforce = parm->setcalcforce;
00330
00331     /*-----*/
00332     /* Added by Michael Grabe */
00333     /*-----*/
00334
00335     thee->zmem = parm->zmem;
00336     thee->setzmem = parm->setzmem;
00337     thee->Lmem = parm->Lmem;
00338     thee->setLmem = parm->setLmem;
00339     thee->mdie = parm->mdie;
00340     thee->setmdie = parm->setmdie;
00341     thee->memv = parm->memv;
00342     thee->setmemv = parm->setmemv;
00343
00344     /*-----*/
00345
00346     thee->numwrite = parm->numwrite;
00347     for (i=0; i<PBEPARM_MAXWRITE; i++) {
00348         thee->writetype[i] = parm->writetype[i];
00349         thee->writefmt[i] = parm->writefmt[i];
00350         for (j=0; j<VMAX_ARGLEN; j++)
00351             thee->writestem[i][j] = parm->writestem[i][j];
00352     }
00353     thee->writemat = parm->writemat;
00354     thee->setwritemat = parm->setwritemat;

```

```

00355     for (i=0; i<VMAX_ARGLEN; i++) thee->writematstem[i] = parm->writematstem[i];
00356     thee->writematflag = parm->writematflag;
00357
00358     thee->smsize = parm->smsize;
00359     thee->smvolume = parm->smvolume;
00360
00361     thee->setsmsize = parm->setsmsize;
00362     thee->setsmvolume = parm->setsmvolume;
00363
00364     thee->parsed = parm->parsed;
00365
00366 }
00367
00368 VPRIVATE int PBEparm_parseLPBE(PBEparm *thee, Vio *sock) {
00369     Vnm_print(0, "Nosh: parsed lpbe\n");
00370     thee->pbetype = PBE_LPBE;
00371     thee->setpbetype = 1;
00372     return 1;
00373 }
00374
00375 VPRIVATE int PBEparm_parseNPBE(PBEparm *thee, Vio *sock) {
00376     Vnm_print(0, "Nosh: parsed npbe\n");
00377     thee->pbetype = PBE_NPBE;
00378     thee->setpbetype = 1;
00379     return 1;
00380 }
00381
00382 VPRIVATE int PBEparm_parseMOL(PBEparm *thee, Vio *sock) {
00383     int ti;
00384     char tok[VMAX_BUFSIZE];
00385
00386     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00387     if (sscanf(tok, "%d", &ti) == 0) {
00388         Vnm_print(2, "Nosh: Read non-int (%s) while parsing MOL \
00389 keyword!\n", tok);
00390         return -1;
00391     }
00392     thee->molid = ti;
00393     thee->setmolid = 1;
00394     return 1;
00395
00396     VERROR1:
00397     Vnm_print(2, "parsePBE: ran out of tokens!\n");
00398     return -1;
00399 }
00400
00401 VPRIVATE int PBEparm_parseLRPBE(PBEparm *thee, Vio *sock) {
00402     Vnm_print(0, "Nosh: parsed lrpbe\n");
00403     thee->pbetype = PBE_LRPBE;
00404     thee->setpbetype = 1;
00405     return 1;
00406 }
00407
00408 VPRIVATE int PBEparm_parseNRPBE(PBEparm *thee, Vio *sock) {
00409     Vnm_print(0, "Nosh: parsed nrpbe\n");
00410     thee->pbetype = PBE_NRPBE;
00411     thee->setpbetype = 1;
00412     return 1;
00413 }
00414
00415 VPRIVATE int PBEparm_parseSMPBE(PBEparm *thee, Vio *sock) {
00416     int i;
00417
00418     char type[VMAX_BUFSIZE]; /* vol or size (keywords) */
00419     char value[VMAX_BUFSIZE]; /* floating point value */
00420
00421     char setVol = 1;
00422     char setSize = 1;
00423     char keyValuePairs = 2;
00424
00425     double size, volume;
00426
00427     for(i=0; i<keyValuePairs; i++){
00428
00429         /* The line two tokens at a time */
00430         VJMPERR1(Vio_scanf(sock, "%s", type) == 1);
00431         VJMPERR1(Vio_scanf(sock, "%s", value) == 1);
00432
00433         if(!strcmp(type, "vol")){
00434             if ((setVol = sscanf(value, "%lf", &volume)) == 0){

```

```

00436         Vnm_print(2,"Nosh: Read non-float (%s) while parsing smpbe keyword!\n", value);
00437         return VRC_FAILURE;
00438     }
00439     }else if(!strcmp(type,"size")){
00440         if ((setSize = sscanf(value, "%lf", &size)) == 0){
00441             Vnm_print(2,"Nosh: Read non-float (%s) while parsing smpbe keyword!\n", value);
00442             return VRC_FAILURE;
00443         }
00444     }else{
00445         Vnm_print(2,"Nosh: Read non-float (%s) while parsing smpbe keyword!\n", value);
00446         return VRC_FAILURE;
00447     }
00448 }
00449
00450 /* If either the volume or size isn't set, throw an error */
00451 if((setVol == 0) || (setSize == 0)){
00452     Vnm_print(2,"Nosh: Error while parsing smpbe keywords! Only size or vol was specified.\n");
00453     return VRC_FAILURE;
00454 }
00455
00456 Vnm_print(0, "Nosh: parsed smpbe\n");
00457 thee->pbetype = PBE_SMPBE;
00458 thee->setpbetype = 1;
00459
00460 thee->smsize = size;
00461 thee->setsmsize = 1;
00462
00463 thee->smvolume = volume;
00464 thee->setsmvolume = 1;
00465
00466 return VRC_SUCCESS;
00467
00468 ERROR1:
00469 Vnm_print(2, "parsePBE: ran out of tokens!\n");
00470 return VRC_FAILURE;
00471
00472 }
00473
00474 VPRIVATE int PBEparm_parseBCFL(PBEparm *thee, Vio *sock) {
00475     char tok[VMAX_BUFSIZE];
00476     int ti;
00477
00478     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00479
00480     /* We can either parse int flag... */
00481     if (sscanf(tok, "%d", &ti) == 1) {
00482
00483         thee->bcfl = (Vbcfl)ti;
00484         thee->setbcfl = 1;
00485         /* Warn that this usage is deprecated */
00486         Vnm_print(2, "parsePBE: Warning -- parsed deprecated \"bcfl %d\" \
00487 statement\n", ti);
00488         Vnm_print(2, "parsePBE: Please use \"bcfl ");
00489         switch (thee->bcfl) {
00490             case BCFL_ZERO:
00491                 Vnm_print(2, "zero");
00492                 break;
00493             case BCFL_SDH:
00494                 Vnm_print(2, "sdh");
00495                 break;
00496             case BCFL_MDH:
00497                 Vnm_print(2, "mdh");
00498                 break;
00499             case BCFL_FOCUS:
00500                 Vnm_print(2, "focus");
00501                 break;
00502             case BCFL_MEM:
00503                 Vnm_print(2, "mem");
00504                 break;
00505             case BCFL_MAP:
00506                 Vnm_print(2, "map");
00507                 break;
00508             default:
00509                 Vnm_print(2, "UNKNOWN");
00510                 break;
00511         }
00512         Vnm_print(2, "\" instead.\n");
00513         return 1;
00514
00515     /* ...or the word */
00516     } else {

```

```

00517
00518     if (Vstring_strcasecmp(tok, "zero") == 0) {
00519         thee->bcfl = BCFL_ZERO;
00520         thee->setbcfl = 1;
00521         return 1;
00522     } else if (Vstring_strcasecmp(tok, "sdh") == 0) {
00523         thee->bcfl = BCFL_SDH;
00524         thee->setbcfl = 1;
00525         return 1;
00526     } else if (Vstring_strcasecmp(tok, "mdh") == 0) {
00527         thee->bcfl = BCFL_MDH;
00528         thee->setbcfl = 1;
00529         return 1;
00530     } else if (Vstring_strcasecmp(tok, "focus") == 0) {
00531         thee->bcfl = BCFL_FOCUS;
00532         thee->setbcfl = 1;
00533         return 1;
00534     } else if (Vstring_strcasecmp(tok, "mem") == 0) {
00535         thee->bcfl = BCFL_MEM;
00536         thee->setbcfl = 1;
00537         return 1;
00538     } else if (Vstring_strcasecmp(tok, "map") == 0) {
00539         thee->bcfl = BCFL_MAP;
00540         thee->setbcfl = 1;
00541         return 1;
00542     } else {
00543         Vnm_print(2, "Nosh:  parsed unknown BCFL parameter (%s)!\n",
00544             tok);
00545         return -1;
00546     }
00547 }
00548 return 0;
00549
00550 ERROR1:
00551     Vnm_print(2, "parsePBE:  ran out of tokens!\n");
00552     return -1;
00553 }
00554
00555 VPRIVATE int PBEparm_parseION(PBEparm *thee, Vio *sock) {
00556
00557     int i;
00558     int meth = 0;
00559
00560     char tok[VMAX_BUFSIZE];
00561     char value[VMAX_BUFSIZE];
00562
00563     double tf;
00564     double charge, conc, radius;
00565
00566     int setCharge = 0;
00567     int setConc = 0;
00568     int setRadius = 0;
00569     int keyValuePairs = 3;
00570
00571     /* Get the initial token for the ION statement */
00572     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00573
00574     /* Scan the token once to determine the type (old style or new key-value pair) */
00575     meth = sscanf(tok, "%lf", &tf);
00576     /* If tok is a non-zero float value, we are using the old method */
00577     if(meth != 0){
00578
00579         Vnm_print(2, "Nosh:  Deprecated use of ION keyword! Use key-value pairs\n", tok);
00580
00581         if (sscanf(tok, "%lf", &tf) == 0) {
00582             Vnm_print(2, "Nosh:  Read non-float (%s) while parsing ION keyword!\n", tok);
00583             return VRC_FAILURE;
00584         }
00585         thee->ionq[thee->nion] = tf;
00586         VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00587         if (sscanf(tok, "%lf", &tf) == 0) {
00588             Vnm_print(2, "Nosh:  Read non-float (%s) while parsing ION keyword!\n", tok);
00589             return VRC_FAILURE;
00590         }
00591         thee->ionc[thee->nion] = tf;
00592         VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00593         if (sscanf(tok, "%lf", &tf) == 0) {
00594             Vnm_print(2, "Nosh:  Read non-float (%s) while parsing ION keyword!\n", tok);
00595             return VRC_FAILURE;
00596         }
00597         thee->ionr[thee->nion] = tf;

```

```

00598
00599     }else{
00600
00601         /* Three key-value pairs (charge, radius and conc) */
00602         for(i=0;i<keyValuePair;i++){
00603
00604             /* Now scan for the value (float) to be used with the key token parsed
00605              * above the if-else statement */
00606             VJMPERR1(Vio_scanf(sock, "%s", value) == 1);
00607             if(!strcmp(tok,"charge")){
00608                 setCharge = sscanf(value, "%lf", &charge);
00609                 if (setCharge == 0){
00610                     Vnm_print(2,"Nosh: Read non-float (%s) while parsing ION %s keyword!\n", value, tok);
00611                     return VRC_FAILURE;
00612                 }
00613                 thee->ionq[thee->nion] = charge;
00614             }else if(!strcmp(tok,"radius")){
00615                 setRadius = sscanf(value, "%lf", &radius);
00616                 if (setRadius == 0){
00617                     Vnm_print(2,"Nosh: Read non-float (%s) while parsing ION %s keyword!\n", value, tok);
00618                     return VRC_FAILURE;
00619                 }
00620                 thee->ionr[thee->nion] = radius;
00621             }else if(!strcmp(tok,"conc")){
00622                 setConc = sscanf(value, "%lf", &conc);
00623                 if (setConc == 0){
00624                     Vnm_print(2,"Nosh: Read non-float (%s) while parsing ION %s keyword!\n", value, tok);
00625                     return VRC_FAILURE;
00626                 }
00627                 thee->ionc[thee->nion] = conc;
00628             }else{
00629                 Vnm_print(2,"Nosh: Illegal or missing key-value pair for ION keyword!\n");
00630                 return VRC_FAILURE;
00631             }
00632
00633             /* If all three values haven't be set (setValue = 0) then read the next token */
00634             if((setCharge != 1) || (setConc != 1) || (setRadius != 1)){
00635                 VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00636             }
00637
00638             } /* end for */
00639         } /* end if */
00640
00641         /* Finally set the setion, nion and setnion flags and return success */
00642         thee->setion[thee->nion] = 1;
00643         (thee->nion)++;
00644         thee->setnion = 1;
00645         return VRC_SUCCESS;
00646
00647     ERROR1:
00648         Vnm_print(2, "parsePBE: ran out of tokens!\n");
00649         return VRC_FAILURE;
00650 }
00651
00652 VPRIVATE int PBEparm_parsePDIE(PBEparm *thee, Vio *sock) {
00653     char tok[VMAX_BUFSIZE];
00654     double tf;
00655
00656     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00657     if (sscanf(tok, "%lf", &tf) == 0) {
00658         Vnm_print(2, "Nosh: Read non-float (%s) while parsing PDIE \
00659 keyword!\n", tok);
00660         return -1;
00661     }
00662     thee->pdie = tf;
00663     thee->setpdie = 1;
00664     return 1;
00665
00666     ERROR1:
00667         Vnm_print(2, "parsePBE: ran out of tokens!\n");
00668         return -1;
00669 }
00670
00671 VPRIVATE int PBEparm_parseSDENS(PBEparm *thee, Vio *sock) {
00672     char tok[VMAX_BUFSIZE];
00673     double tf;
00674
00675     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00676     if (sscanf(tok, "%lf", &tf) == 0) {
00677         Vnm_print(2, "Nosh: Read non-float (%s) while parsing SDENS \
00678 keyword!\n", tok);

```

```

00679         return -1;
00680     }
00681     thee->sdens = tf;
00682     thee->setsdens = 1;
00683     return 1;
00684
00685     ERROR1:
00686     Vnm_print(2, "parsePBE: ran out of tokens!\n");
00687     return -1;
00688 }
00689
00690 VPRIVATE int PBEparm_parseSDIE(PBEparm *thee, Vio *sock) {
00691     char tok[VMAX_BUFSIZE];
00692     double tf;
00693
00694     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00695     if (sscanf(tok, "%lf", &tf) == 0) {
00696         Vnm_print(2, "NOsh: Read non-float (%s) while parsing SDIE \
00697 keyword!\n", tok);
00698         return -1;
00699     }
00700     thee->sdie = tf;
00701     thee->setsdie = 1;
00702     return 1;
00703
00704     ERROR1:
00705     Vnm_print(2, "parsePBE: ran out of tokens!\n");
00706     return -1;
00707 }
00708
00709 VPRIVATE int PBEparm_parseSRFM(PBEparm *thee, Vio *sock) {
00710     char tok[VMAX_BUFSIZE];
00711     int ti;
00712
00713     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00714
00715     /* Parse old-style int arg */
00716     if (sscanf(tok, "%d", &ti) == 1) {
00717         thee->srfm = (Vsurf_Meth)ti;
00718         thee->setsrfm = 1;
00719
00720         Vnm_print(2, "parsePBE: Warning -- parsed deprecated \"srfm %d\" \
00721 statement.\n", ti);
00722         Vnm_print(2, "parsePBE: Please use \"srfm ");
00723         switch (thee->srfm) {
00724             case VSM_MOL:
00725                 Vnm_print(2, "mol");
00726                 break;
00727             case VSM_MOLSMOOTH:
00728                 Vnm_print(2, "smol");
00729                 break;
00730             case VSM_SPLINE:
00731                 Vnm_print(2, "spl2");
00732                 break;
00733             case VSM_SPLINE3:
00734                 Vnm_print(2, "spl3");
00735                 break;
00736             case VSM_SPLINE4:
00737                 Vnm_print(2, "spl4");
00738                 break;
00739             default:
00740                 Vnm_print(2, "UNKNOWN");
00741                 break;
00742         }
00743         Vnm_print(2, "\" instead.\n");
00744         return 1;
00745
00746         /* Parse newer text-based args */
00747     } else if (Vstring_strcasecmp(tok, "mol") == 0) {
00748         thee->srfm = VSM_MOL;
00749         thee->setsrfm = 1;
00750         return 1;
00751     } else if (Vstring_strcasecmp(tok, "smol") == 0) {
00752         thee->srfm = VSM_MOLSMOOTH;
00753         thee->setsrfm = 1;
00754         return 1;
00755     } else if (Vstring_strcasecmp(tok, "spl2") == 0) {
00756         thee->srfm = VSM_SPLINE;
00757         thee->setsrfm = 1;
00758         return 1;
00759     } else if (Vstring_strcasecmp(tok, "spl3") == 0) {

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```

00760     thee->srfm = VSM_SPLINE3;
00761     thee->setsrfm = 1;
00762     return 1;
00763 } else if (Vstring_strcasecmp(tok, "spl4") == 0) {
00764     thee->srfm = VSM_SPLINE4;
00765     thee->setsrfm = 1;
00766     return 1;
00767 } else {
00768     Vnm_print(2, "Nosh: Unrecongized keyword (%s) when parsing \
00769 srfm!\n", tok);
00770     return -1;
00771 }
00772 return 0;
00773
00774 ERROR1:
00775     Vnm_print(2, "parsePBE: ran out of tokens!\n");
00776     return -1;
00777 }
00778 }
00779
00780 VPRIVATE int PBEparm_parseSRAD(PBEparm *thee, Vio *sock) {
00781     char tok[VMAX_BUFSIZE];
00782     double tf;
00783
00784     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00785     if (sscanf(tok, "%lf", &tf) == 0) {
00786         Vnm_print(2, "Nosh: Read non-float (%s) while parsing SRAD \
00787 keyword!\n", tok);
00788         return -1;
00789     }
00790     thee->srاد = tf;
00791     thee->setsrad = 1;
00792     return 1;
00793
00794 ERROR1:
00795     Vnm_print(2, "parsePBE: ran out of tokens!\n");
00796     return -1;
00797 }
00798
00799 VPRIVATE int PBEparm_parseSWIN(PBEparm *thee, Vio *sock) {
00800     char tok[VMAX_BUFSIZE];
00801     double tf;
00802
00803     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00804     if (sscanf(tok, "%lf", &tf) == 0) {
00805         Vnm_print(2, "Nosh: Read non-float (%s) while parsing SWIN \
00806 keyword!\n", tok);
00807         return -1;
00808     }
00809     thee->swin = tf;
00810     thee->setswin = 1;
00811     return 1;
00812
00813 ERROR1:
00814     Vnm_print(2, "parsePBE: ran out of tokens!\n");
00815     return -1;
00816 }
00817
00818 VPRIVATE int PBEparm_parseTEMP(PBEparm *thee, Vio *sock) {
00819     char tok[VMAX_BUFSIZE];
00820     double tf;
00821
00822     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00823     if (sscanf(tok, "%lf", &tf) == 0) {
00824         Vnm_print(2, "Nosh: Read non-float (%s) while parsing TEMP \
00825 keyword!\n", tok);
00826         return -1;
00827     }
00828     thee->temp = tf;
00829     thee->settemp = 1;
00830     return 1;
00831
00832 ERROR1:
00833     Vnm_print(2, "parsePBE: ran out of tokens!\n");
00834     return -1;
00835 }
00836
00837 VPRIVATE int PBEparm_parseUSEMAP(PBEparm *thee, Vio *sock) {
00838     char tok[VMAX_BUFSIZE];
00839     int ti;
00840

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00841     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00842     Vnm_print(0, "PBEparm_parseToken: Read %s...\n", tok);
00843     if (Vstring_strcasecmp(tok, "diel") == 0) {
00844         thee->useDielMap = 1;
00845         VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00846         if (sscanf(tok, "%d", &ti) == 0) {
00847             Vnm_print(2, "Nosh: Read non-int (%s) while parsing \
00848 USEMAP DIEL keyword!\n", tok);
00849             return -1;
00850         }
00851         thee->dielMapID = ti;
00852         return 1;
00853     } else if (Vstring_strcasecmp(tok, "kappa") == 0) {
00854         thee->useKappaMap = 1;
00855         VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00856         if (sscanf(tok, "%d", &ti) == 0) {
00857             Vnm_print(2, "Nosh: Read non-int (%s) while parsing \
00858 USEMAP KAPPA keyword!\n", tok);
00859             return -1;
00860         }
00861         thee->kappaMapID = ti;
00862         return 1;
00863     } else if (Vstring_strcasecmp(tok, "pot") == 0) {
00864         thee->usePotMap = 1;
00865         VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00866         if (sscanf(tok, "%d", &ti) == 0) {
00867             Vnm_print(2, "Nosh: Read non-int (%s) while parsing \
00868 USEMAP POT keyword!\n", tok);
00869             return -1;
00870         }
00871         thee->potMapID = ti;
00872         return 1;
00873     } else if (Vstring_strcasecmp(tok, "charge") == 0) {
00874         thee->useChargeMap = 1;
00875         VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00876         if (sscanf(tok, "%d", &ti) == 0) {
00877             Vnm_print(2, "Nosh: Read non-int (%s) while parsing \
00878 USEMAP CHARGE keyword!\n", tok);
00879             return -1;
00880         }
00881         thee->chargeMapID = ti;
00882         return 1;
00883     } else {
00884         Vnm_print(2, "Nosh: Read undefined keyword (%s) while parsing \
00885 USEMAP statement!\n", tok);
00886         return -1;
00887     }
00888     return 0;
00889
00890     ERROR1:
00891     Vnm_print(2, "parsePBE: ran out of tokens!\n");
00892     return -1;
00893 }
00894
00895 VPRIVATE int PBEparm_parseCALCENERGY(PBEparm *thee, Vio *sock) {
00896     char tok[VMAX_BUFSIZE];
00897     int ti;
00898
00899     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00900     /* Parse number */
00901     if (sscanf(tok, "%d", &ti) == 1) {
00902         thee->calcenergy = (PBEparm_calcEnergy)ti;
00903         thee->setcalcenergy = 1;
00904
00905         Vnm_print(2, "parsePBE: Warning -- parsed deprecated \"calcenergy \
00906 %d\" statement.\n", ti);
00907         Vnm_print(2, "parsePBE: Please use \"calcenergy ");
00908         switch (thee->calcenergy) {
00909             case PCE_NO:
00910                 Vnm_print(2, "no");
00911                 break;
00912             case PCE_TOTAL:
00913                 Vnm_print(2, "total");
00914                 break;
00915             case PCE_COMPS:
00916                 Vnm_print(2, "comps");
00917                 break;
00918             default:
00919                 Vnm_print(2, "UNKNOWN");
00920                 break;
00921         }

```



```

00922     Vnm_print(2, "\" instead.\n");
00923     return 1;
00924 } else if (Vstring_strcasecmp(tok, "no") == 0) {
00925     thee->calcenergy = PCE_NO;
00926     thee->setcalcenergy = 1;
00927     return 1;
00928 } else if (Vstring_strcasecmp(tok, "total") == 0) {
00929     thee->calcenergy = PCE_TOTAL;
00930     thee->setcalcenergy = 1;
00931     return 1;
00932 } else if (Vstring_strcasecmp(tok, "comps") == 0) {
00933     thee->calcenergy = PCE_COMPS;
00934     thee->setcalcenergy = 1;
00935     return 1;
00936 } else {
00937     Vnm_print(2, "Nosh: Unrecognized parameter (%s) while parsing \
00938 calcenergy!\n", tok);
00939     return -1;
00940 }
00941 return 0;
00942
00943 ERROR1:
00944     Vnm_print(2, "parsePBE: ran out of tokens!\n");
00945     return -1;
00946 }
00947
00948 VPRIVATE int PBEparm_parseCALCFORCE(PBEparm *thee, Vio *sock) {
00949     char tok[VMAX_BUFSIZE];
00950     int ti;
00951
00952     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00953     /* Parse number */
00954     if (sscanf(tok, "%d", &ti) == 1) {
00955         thee->calcforce = (PBEparm_calcForce)ti;
00956         thee->setcalcforce = 1;
00957
00958         Vnm_print(2, "parsePBE: Warning -- parsed deprecated \"calcforce \
00959 %d\" statement.\n", ti);
00960         Vnm_print(2, "parsePBE: Please use \"calcforce ");
00961         switch (thee->calcenergy) {
00962             case PCF_NO:
00963                 Vnm_print(2, "no");
00964                 break;
00965             case PCF_TOTAL:
00966                 Vnm_print(2, "total");
00967                 break;
00968             case PCF_COMPS:
00969                 Vnm_print(2, "comps");
00970                 break;
00971             default:
00972                 Vnm_print(2, "UNKNOWN");
00973                 break;
00974         }
00975         Vnm_print(2, "\" instead.\n");
00976         return 1;
00977     } else if (Vstring_strcasecmp(tok, "no") == 0) {
00978         thee->calcforce = PCF_NO;
00979         thee->setcalcforce = 1;
00980         return 1;
00981     } else if (Vstring_strcasecmp(tok, "total") == 0) {
00982         thee->calcforce = PCF_TOTAL;
00983         thee->setcalcforce = 1;
00984         return 1;
00985     } else if (Vstring_strcasecmp(tok, "comps") == 0) {
00986         thee->calcforce = PCF_COMPS;
00987         thee->setcalcforce = 1;
00988         return 1;
00989     } else {
00990         Vnm_print(2, "Nosh: Unrecognized parameter (%s) while parsing \
00991 calcforce!\n", tok);
00992         return -1;
00993     }
00994     return 0;
00995
00996 ERROR1:
00997     Vnm_print(2, "parsePBE: ran out of tokens!\n");
00998     return -1;
00999 }
01000
01001 /*-----*/
01002 /* Added by Michael Grabe */

```

```

01003 /*-----*/
01004
01005 VPRIVATE int PBEparm_parseZMEM(PBEparm *thee, Vio *sock) {
01006     char tok[VMAX_BUFSIZE];
01007     double tf;
01008
01009     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
01010     if (sscanf(tok, "%lf", &tf) == 0) {
01011         Vnm_print(2, "Nosh: Read non-float (%s) while parsing ZMEM \
01012             keyword!\n", tok);
01013         return -1;
01014     }
01015     thee->zmem = tf;
01016     thee->setzmem = 1;
01017     return 1;
01018
01019 ERROR1:
01020     Vnm_print(2, "parsePBE: ran out of tokens!\n");
01021     return -1;
01022 }
01023
01024
01025 VPRIVATE int PBEparm_parseLMEM(PBEparm *thee, Vio *sock) {
01026     char tok[VMAX_BUFSIZE];
01027     double tf;
01028
01029     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
01030     if (sscanf(tok, "%lf", &tf) == 0) {
01031         Vnm_print(2, "Nosh: Read non-float (%s) while parsing LMEM \
01032             keyword!\n", tok);
01033         return -1;
01034     }
01035     thee->lmem = tf;
01036     thee->setlmem = 1;
01037     return 1;
01038
01039 ERROR1:
01040     Vnm_print(2, "parsePBE: ran out of tokens!\n");
01041     return -1;
01042 }
01043
01044 VPRIVATE int PBEparm_parseMDIE(PBEparm *thee, Vio *sock) {
01045     char tok[VMAX_BUFSIZE];
01046     double tf;
01047
01048     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
01049     if (sscanf(tok, "%lf", &tf) == 0) {
01050         Vnm_print(2, "Nosh: Read non-float (%s) while parsing MDIE \
01051             keyword!\n", tok);
01052         return -1;
01053     }
01054     thee->mdie = tf;
01055     thee->setmdie = 1;
01056     return 1;
01057
01058 ERROR1:
01059     Vnm_print(2, "parsePBE: ran out of tokens!\n");
01060     return -1;
01061 }
01062
01063 VPRIVATE int PBEparm_parseMEMV(PBEparm *thee, Vio *sock) {
01064     char tok[VMAX_BUFSIZE];
01065     double tf;
01066
01067     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
01068     if (sscanf(tok, "%lf", &tf) == 0) {
01069         Vnm_print(2, "Nosh: Read non-float (%s) while parsing MEMV \
01070             keyword!\n", tok);
01071         return -1;
01072     }
01073     thee->memv = tf;
01074     thee->setmemv = 1;
01075     return 1;
01076
01077 ERROR1:
01078     Vnm_print(2, "parsePBE: ran out of tokens!\n");
01079     return -1;
01080 }
01081
01082 /*-----*/
01083

```

```

01084 VPRIVATE int PBEparm_parseWRITE(PBEparm *thee, Vio *sock) {
01085     char tok[VMAX_BUFSIZE], str[VMAX_BUFSIZE]="", strnew[VMAX_BUFSIZE]="";
01086     Vdata_Type writetype;
01087     Vdata_Format writefmt;
01088
01089     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
01090     if (Vstring_strcasecmp(tok, "pot") == 0) {
01091         writetype = VDT_POT;
01092     } else if (Vstring_strcasecmp(tok, "atompot") == 0) {
01093         writetype = VDT_ATOMPOT;
01094     } else if (Vstring_strcasecmp(tok, "charge") == 0) {
01095         writetype = VDT_CHARGE;
01096     } else if (Vstring_strcasecmp(tok, "smol") == 0) {
01097         writetype = VDT_SMOL;
01098     } else if (Vstring_strcasecmp(tok, "dielx") == 0) {
01099         writetype = VDT_DIELX;
01100     } else if (Vstring_strcasecmp(tok, "diely") == 0) {
01101         writetype = VDT_DIELY;
01102     } else if (Vstring_strcasecmp(tok, "dielz") == 0) {
01103         writetype = VDT_DIELZ;
01104     } else if (Vstring_strcasecmp(tok, "kappa") == 0) {
01105         writetype = VDT_KAPPA;
01106     } else if (Vstring_strcasecmp(tok, "sspl") == 0) {
01107         writetype = VDT_SSPL;
01108     } else if (Vstring_strcasecmp(tok, "vdw") == 0) {
01109         writetype = VDT_VDW;
01110     } else if (Vstring_strcasecmp(tok, "ivdw") == 0) {
01111         writetype = VDT_IVDW;
01112     } else if (Vstring_strcasecmp(tok, "lap") == 0) {
01113         writetype = VDT_LAP;
01114     } else if (Vstring_strcasecmp(tok, "edens") == 0) {
01115         writetype = VDT_EDENS;
01116     } else if (Vstring_strcasecmp(tok, "ndens") == 0) {
01117         writetype = VDT_NDENS;
01118     } else if (Vstring_strcasecmp(tok, "qdens") == 0) {
01119         writetype = VDT_QDENS;
01120     } else if (Vstring_strcasecmp(tok, "3dmap") == 0) {
01121         VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
01122         strcpy(thee->pbam_3dmapstem, tok);
01123         thee->pbam_3dmapflag = 1;
01124         return 1;
01125     } else {
01126         Vnm_print(2, "PBEparm_parse: Invalid data type (%s) to write!\n",
01127             tok);
01128         return -1;
01129     }
01130
01131     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
01132     if (Vstring_strcasecmp(tok, "dx") == 0) {
01133         writefmt = VDF_DX;
01134     }
01135     else if (Vstring_strcasecmp(tok, "dxbin") == 0) {
01136         writefmt = VDF_DXBIN;
01137     } else if (Vstring_strcasecmp(tok, "uhbd") == 0) {
01138         writefmt = VDF_UHBD;
01139     } else if (Vstring_strcasecmp(tok, "avs") == 0) {
01140         writefmt = VDF_AVIS;
01141     } else if (Vstring_strcasecmp(tok, "gz") == 0) {
01142         writefmt = VDF_GZ;
01143     } else if (Vstring_strcasecmp(tok, "flat") == 0) {
01144         writefmt = VDF_FLAT;
01145     } else {
01146         Vnm_print(2, "PBEparm_parse: Invalid data format (%s) to write!\n",
01147             tok);
01148         return -1;
01149     }
01150     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
01151     if (tok[0]!=' ') {
01152         strcpy(strnew, "");
01153         while (tok[strlen(tok)-1] != ' ') {
01154             strcat(str, tok);
01155             strcat(str, " ");
01156             VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
01157         }
01158         strcat(str, tok);
01159         strncpy(strnew, str+1, strlen(str)-2);
01160         strcpy(tok, strnew);
01161     }
01162     if (thee->numwrite < (PBEPARM_MAXWRITE-1)) {
01163         strncpy(thee->writestem[thee->numwrite], tok, VMAX_ARGLEN);
01164         thee->writetype[thee->numwrite] = writetype;

```

```

01165         thee->writefmt[thee->numwrite] = writefmt;
01166         (thee->numwrite)++;
01167     } else {
01168         Vnm_print(2, "PBEparm_parse: You have exceeded the maximum number of write statements!\n");
01169         Vnm_print(2, "PBEparm_parse: Ignoring additional write statements!\n");
01170     }
01171     return 1;
01172
01173     VERROR1:
01174         Vnm_print(2, "parsePBE: ran out of tokens!\n");
01175         return -1;
01176 }
01177
01178 VPRIVATE int PBEparm_parseWRITEMAT(PBEparm *thee, Vio *sock) {
01179     char tok[VMAX_BUFSIZE], str[VMAX_BUFSIZE]="", strnew[VMAX_BUFSIZE]="";
01180
01181     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
01182     if (Vstring_strcasecmp(tok, "poisson") == 0) {
01183         thee->writematflag = 0;
01184     } else if (Vstring_strcasecmp(tok, "full") == 0) {
01185         thee->writematflag = 1;
01186     } else {
01187         Vnm_print(2, "Nosh: Invalid format (%s) while parsing \
01188 WRITEMAT keyword!\n", tok);
01189         return -1;
01190     }
01191
01192     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
01193     if (tok[0]!=' ') {
01194         strcpy(strnew, "");
01195         while (tok[strlen(tok)-1] != ' ') {
01196             strcat(str, tok);
01197             strcat(str, " ");
01198             VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
01199         }
01200         strcat(str, tok);
01201         strncpy(strnew, str+1, strlen(str)-2);
01202         strcpy(tok, strnew);
01203     }
01204     strncpy(thee->writematstem, tok, VMAX_ARGLEN);
01205     thee->setwritemat = 1;
01206     thee->writemat = 1;
01207     return 1;
01208
01209     VERROR1:
01210         Vnm_print(2, "parsePBE: ran out of tokens!\n");
01211         return -1;
01212
01213 }
01214
01215 VPUBLIC int PBEparm_parseToken(PBEparm *thee, char tok[VMAX_BUFSIZE],
01216 Vio *sock) {
01217     if (thee == VNULL) {
01218         Vnm_print(2, "parsePBE: got NULL thee!\n");
01219         return -1;
01220     }
01221     if (sock == VNULL) {
01222         Vnm_print(2, "parsePBE: got NULL socket!\n");
01223         return -1;
01224     }
01225
01226     Vnm_print(0, "PBEparm_parseToken: trying %s...\n", tok);
01227
01228     if (Vstring_strcasecmp(tok, "mol") == 0) {
01229         return PBEparm_parseMOL(thee, sock);
01230     } else if (Vstring_strcasecmp(tok, "lpbe") == 0) {
01231         return PBEparm_parseLPBE(thee, sock);
01232     } else if (Vstring_strcasecmp(tok, "npbe") == 0) {
01233         return PBEparm_parseNPBE(thee, sock);
01234     } else if (Vstring_strcasecmp(tok, "lrpbe") == 0) {
01235         return PBEparm_parseLRPBE(thee, sock);
01236     } else if (Vstring_strcasecmp(tok, "nrpbe") == 0) {
01237         return PBEparm_parseNRPBE(thee, sock);
01238     } else if (Vstring_strcasecmp(tok, "smpbe") == 0) {
01239         return PBEparm_parseSMPBE(thee, sock);
01240     } else if (Vstring_strcasecmp(tok, "bcfl") == 0) {
01241         return PBEparm_parseBCFL(thee, sock);
01242     } else if (Vstring_strcasecmp(tok, "ion") == 0) {
01243         return PBEparm_parseION(thee, sock);
01244     } else if (Vstring_strcasecmp(tok, "pdie") == 0) {

```

```

01246     return PBEparm_parsePDIE(thee, sock);
01247 } else if (Vstring_strcasecmp(tok, "sdens") == 0) {
01248     return PBEparm_parseSDENS(thee, sock);
01249 } else if (Vstring_strcasecmp(tok, "sdie") == 0) {
01250     return PBEparm_parseSDIE(thee, sock);
01251 } else if (Vstring_strcasecmp(tok, "srfm") == 0) {
01252     return PBEparm_parseSRFM(thee, sock);
01253 } else if (Vstring_strcasecmp(tok, "srad") == 0) {
01254     return PBEparm_parseSRAD(thee, sock);
01255 } else if (Vstring_strcasecmp(tok, "swin") == 0) {
01256     return PBEparm_parseSWIN(thee, sock);
01257 } else if (Vstring_strcasecmp(tok, "temp") == 0) {
01258     return PBEparm_parseTEMP(thee, sock);
01259 } else if (Vstring_strcasecmp(tok, "usemap") == 0) {
01260     return PBEparm_parseUSEMAP(thee, sock);
01261 } else if (Vstring_strcasecmp(tok, "calcenergy") == 0) {
01262     return PBEparm_parseCALCENERGY(thee, sock);
01263 } else if (Vstring_strcasecmp(tok, "calcforce") == 0) {
01264     return PBEparm_parseCALCFORCE(thee, sock);
01265 } else if (Vstring_strcasecmp(tok, "write") == 0) {
01266     return PBEparm_parseWRITE(thee, sock);
01267 } else if (Vstring_strcasecmp(tok, "writemat") == 0) {
01268     return PBEparm_parseWRITEMAT(thee, sock);
01269
01270 /*-----*/
01271 /* Added by Michael Grabe */
01272 /*-----*/
01273
01274 } else if (Vstring_strcasecmp(tok, "zmem") == 0) {
01275     return PBEparm_parseZMEM(thee, sock);
01276 } else if (Vstring_strcasecmp(tok, "lmem") == 0) {
01277     return PBEparm_parseLMEM(thee, sock);
01278 } else if (Vstring_strcasecmp(tok, "mdie") == 0) {
01279     return PBEparm_parseMDIE(thee, sock);
01280 } else if (Vstring_strcasecmp(tok, "memv") == 0) {
01281     return PBEparm_parseMEMV(thee, sock);
01282 }
01283
01284 /*-----*/
01285
01286     return 0;
01287
01288 }

```

9.44 src/generic/pbeparm.h File Reference

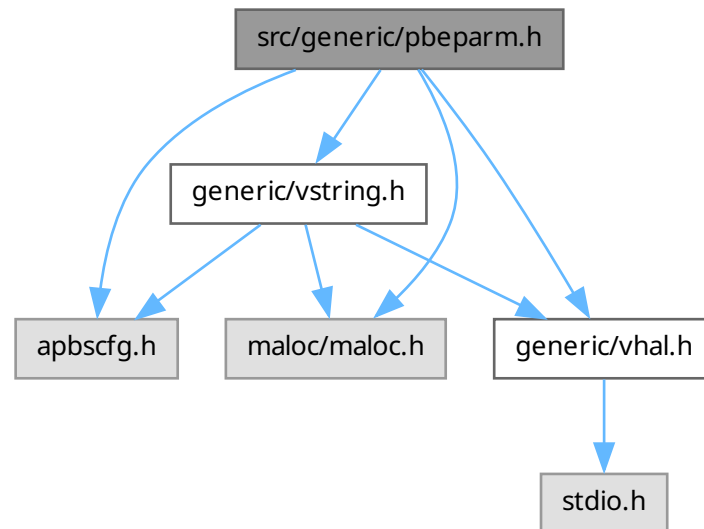
Contains declarations for class PBEparm.

```

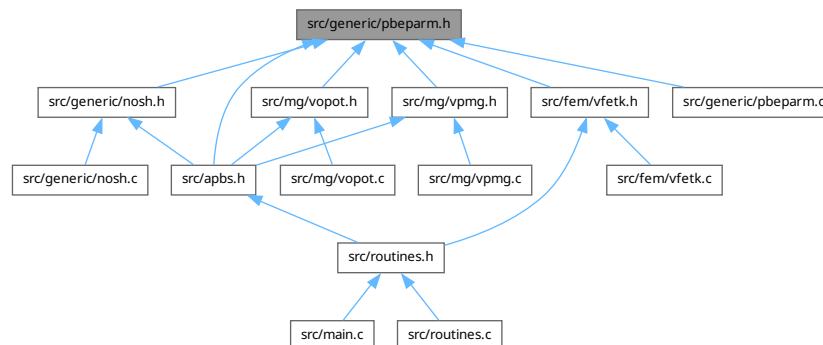
#include "apbscfg.h"
#include "malloc/malloc.h"
#include "generic/vhal.h"
#include "generic/vstring.h"

```

Include dependency graph for pbeparm.h:



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [SPBEparam](#)

Parameter structure for PBE variables from input files.

Macros

- #define [PBEPARM_MAXWRITE](#) 20

Number of things that can be written out in a single calculation.

Typedefs

- typedef enum [ePBEparm_calcEnergy](#) [PBEparm_calcEnergy](#)
Define ePBEparm_calcEnergy enumeration as PBEparm_calcEnergy.
- typedef enum [ePBEparm_calcForce](#) [PBEparm_calcForce](#)
Define ePBEparm_calcForce enumeration as PBEparm_calcForce.
- typedef struct [sPBEparm](#) [PBEparm](#)
Declaration of the PBEparm class as the PBEparm structure.

Enumerations

- enum [ePBEparm_calcEnergy](#) { [PCE_NO](#) =0 , [PCE_TOTAL](#) =1 , [PCE_COMPS](#) =2 }
Define energy calculation enumeration.
- enum [ePBEparm_calcForce](#) { [PCF_NO](#) =0 , [PCF_TOTAL](#) =1 , [PCF_COMPS](#) =2 }
Define force calculation enumeration.

Functions

- VEXTERNC double [PBEparm_getIonCharge](#) ([PBEparm](#) *thee, int iion)
Get charge (e) of specified ion species.
- VEXTERNC double [PBEparm_getIonConc](#) ([PBEparm](#) *thee, int iion)
Get concentration (M) of specified ion species.
- VEXTERNC double [PBEparm_getIonRadius](#) ([PBEparm](#) *thee, int iion)
Get radius (Å) of specified ion species.
- VEXTERNC [PBEparm](#) * [PBEparm_ctor](#) ()
Construct PBEparm object.
- VEXTERNC int [PBEparm_ctor2](#) ([PBEparm](#) *thee)
FORTTRAN stub to construct PBEparm object.
- VEXTERNC void [PBEparm_dtor](#) ([PBEparm](#) **thee)
Object destructor.
- VEXTERNC void [PBEparm_dtor2](#) ([PBEparm](#) *thee)
FORTTRAN stub for object destructor.
- VEXTERNC int [PBEparm_check](#) ([PBEparm](#) *thee)
Consistency check for parameter values stored in object.
- VEXTERNC void [PBEparm_copy](#) ([PBEparm](#) *thee, [PBEparm](#) *parm)
Copy PBEparm object into thee.
- VEXTERNC int [PBEparm_parseToken](#) ([PBEparm](#) *thee, char tok[VMAX_BUFSIZE], Vio *sock)
Parse a keyword from an input file.

9.44.1 Detailed Description

Contains declarations for class PBEparm.

Version

\$Id\$

Author

Nathan A. Baker

Attention

```

*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
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* Pacific Northwest National Laboratory
*
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*
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* THE POSSIBILITY OF SUCH DAMAGE.
*
*

```

Definition in file [pbeparm.h](#).

9.45 pbeparm.h

[Go to the documentation of this file.](#)

```

00001
00062 #ifndef _PBEPARM_H_
00063 #define _PBEPARM_H_
00064
00065 #include "apbscfg.h"
00066
00067 #include "malloc/malloc.h"
00068
00069 #include "generic/vhal.h"
00070 #include "generic/vstring.h"
00071
00075 #define PBEPARM_MAXWRITE 20
00076
00081 enum ePBEParm_calcEnergy {
00082     PCE_NO=0,

```



```

00083     PCE_TOTAL=1,
00084     PCE_COMPS=2
00085 };
00086
00091 typedef enum ePBEParm_calcEnergy PBEParm_calcEnergy;
00092
00097 enum ePBEParm_calcForce {
00098     PCF_NO=0,
00099     PCF_TOTAL=1,
00100     PCF_COMPS=2
00101 };
00102
00107 typedef enum ePBEParm_calcForce PBEParm_calcForce;
00108
00117 struct sPBEParm {
00118
00119     int molid;
00120     int setmolid;
00121     int useDielMap;
00123     int dielMapID;
00124     int useKappaMap;
00126     int kappaMapID;
00127     int usePotMap;
00129     int potMapID;
00131     int useChargeMap;
00133     int chargeMapID;
00134     Vhal_PBEType pbetype;
00135     int setpbetype;
00136     Vbcfl bcfl;
00137     int setbcfl;
00138     int nion;
00139     int setnion;
00140     double ionq[MAXION];
00141     double ionc[MAXION];
00142     double ionr[MAXION];
00143     int setion[MAXION];
00144     double pdie;
00145     int setpdie;
00146     double sdens;
00147     int setsdens;
00148     double sdie;
00149     int setsdie;
00150     Vsurf_Meth srfm;
00151     int setsrfm;
00152     double srad;
00153     int setsrad;
00154     double swin;
00155     int setswin;
00156     double temp;
00157     int settemp;
00159     double smsize;
00160     int setsmsize;
00162     double smvolume;
00163     int setsmvolume;
00165     PBEParm_calcEnergy calcenergy;
00166     int setcalcenergy;
00167     PBEParm_calcForce calcforce;
00168     int setcalcforce;
00170     /*-----*/
00171     /* Added by Michael Grabe */
00172     /*-----*/
00173
00174     double zmem;
00175     int setzmem;
00176     double lmem;
00177     int setlmem;
00178     double mdie;
00179     int setmdie;
00180     double memv;
00181     int setmemv;
00183     /*-----*/
00184
00185     int numwrite;
00186     char writestem[PBEPARM_MAXWRITE][VMAX_ARGLEN];
00188     Vdata_Type writetype[PBEPARM_MAXWRITE];
00189     Vdata_Format writefmt[PBEPARM_MAXWRITE];
00191     int writemat;
00194     int setwritemat;
00195     char writematstem[VMAX_ARGLEN];
00196     int writematflag;
00201 /*Added for issue 482*/

```

```

00202 char pbam_3dmapstem[VMAX_ARGLEN];
00203 int pbam_3dmapflag;
00204
00205     int parsed;
00207 };
00208
00213 typedef struct sPBEParm PBEParm;
00214
00215 /* ////////////////////////////////////////
00216 // Class NOsh: Non-inlineable methods (mcsh.c)
00218
00224 VEXTERNC double PBEParm_getIonCharge(
00225     PBEParm *thee, /**< PBEParm object */
00226     int iion
00227 );
00228
00234 VEXTERNC double PBEParm_getIonConc(
00235     PBEParm *thee,
00236     int iion
00237 );
00238
00244 VEXTERNC double PBEParm_getIonRadius(
00245     PBEParm *thee,
00246     int iion
00247 );
00248
00249
00255 VEXTERNC PBEParm* PBEParm_ctor();
00256
00262 VEXTERNC int PBEParm_ctor2(
00263     PBEParm *thee
00264 );
00265
00270 VEXTERNC void PBEParm_dtor(
00271     PBEParm **thee
00272 );
00273
00278 VEXTERNC void PBEParm_dtor2(
00279     PBEParm *thee
00280 );
00281
00287 VEXTERNC int PBEParm_check(
00288     PBEParm *thee
00289 );
00290
00295 VEXTERNC void PBEParm_copy(
00296     PBEParm *thee,
00297     PBEParm *parm
00298 );
00299
00306 VEXTERNC int PBEParm_parseToken(
00307     PBEParm *thee,
00308     char tok[VMAX_BUFSIZE],
00309     Vio *sock
00310 );
00311
00312
00313 #endif
00314

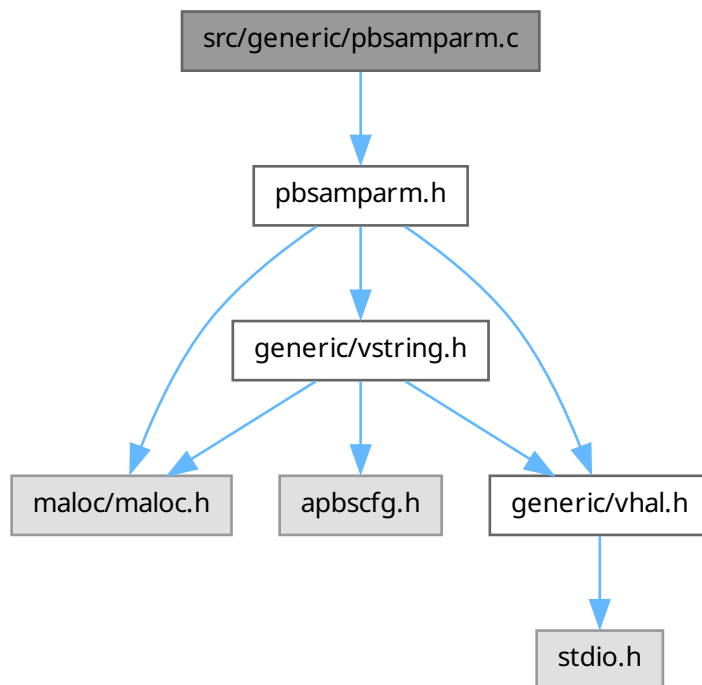
```

9.46 src/generic/pbsamparm.c File Reference

Class PBSAMparm methods.

```
#include "pbsamparm.h"
```

Include dependency graph for pbsamparm.c:



Functions

- VPUBLIC PBSAMparm * PBSAMparm_ctor (PBSAMparm_CalcType type)
Construct PBSAMparm object.
- VPUBLIC Vrc_Codes PBSAMparm_ctor2 (PBSAMparm *thee, PBSAMparm_CalcType type)
FORTTRAN stub to construct PBSAMparm object ??????????!!!!!!
- VPUBLIC void PBSAMparm_dtor (PBSAMparm **thee)
Object destructor.
- VPUBLIC void PBSAMparm_dtor2 (PBSAMparm *thee)
FORTTRAN stub for object destructor ??????????!!!!!!
- VPUBLIC Vrc_Codes PBSAMparm_check (PBSAMparm *thee)
Consistency check for parameter values stored in object.
- VPUBLIC void PBSAMparm_copy (PBSAMparm *thee, PBSAMparm *parm)
copy PBSAMparm object into thee.
- VPRIVATE Vrc_Codes PBSAMparm_parseSurf (PBSAMparm *thee, Vio *sock)
Find vertex files for each molecule and save them.
- VPRIVATE Vrc_Codes PBSAMparm_parseMSMS (PBSAMparm *thee, Vio *sock)
Find msms flag for if MSMS is to be run.
- VPRIVATE Vrc_Codes PBSAMparm_parselmat (PBSAMparm *thee, Vio *sock)

Find IMAT files for each molecule and save them.

- VPRIVATE Vrc_Codes [PBSAMparm_parseExp](#) ([PBSAMparm](#) *thee, Vio *sock)

Find expansion files for each molecule and save them.

- VPRIVATE Vrc_Codes [PBSAMparm_parseTolsp](#) ([PBSAMparm](#) *thee, Vio *sock)

Find sphere tolerance for coarse-graining.

- VPUBLIC Vrc_Codes [PBSAMparm_parseToken](#) ([PBSAMparm](#) *thee, char tok[VMAX_BUFSIZE], Vio *sock)

Parse an MG keyword from an input file.

9.46.1 Detailed Description

Class PBSAMparm methods.

Author

Andrew Stevens

Version

\$Id\$

Attention

```
*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
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*   Pacific Northwest National Laboratory
*
*   Additional contributing authors listed in the code documentation.
*
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```

```

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* THE POSSIBILITY OF SUCH DAMAGE.
*
*

```

Definition in file [pbsamparm.c](#).

9.47 pbsamparm.c

[Go to the documentation of this file.](#)

```

00001
00057 #include "pbsamparm.h"
00058
00059 VEMBED(rcsid="$Id$")
00060
00061 #if !defined(VINLINE_MGPARM)
00062
00063 #endif /* if !defined(VINLINE_MGPARM) */
00064
00065
00066 VPUBLIC PBSAMParm* PBSAMParm_ctor(PBSAMParm_CalcType type) {
00067
00068     /* Set up the structure */
00069     PBSAMParm *thee = VNULL;
00070     thee = (PBSAMParm*)Vmem_malloc(VNULL, 1, sizeof(PBSAMParm));
00071     VASSERT( thee != VNULL);
00072     VASSERT( PBSAMParm_ctor2(thee, type) == VRC_SUCCESS );
00073
00074     return thee;
00075 }
00076
00077 VPUBLIC Vrc_Codes PBSAMParm_ctor2(PBSAMParm *thee, PBSAMParm_CalcType type) {
00078
00079     int i;
00080
00081     if (thee == VNULL) return VRC_FAILURE;
00082
00083     thee->tolsp = 2.5;
00084     thee->setmsms = 0;
00085     thee->probe_radius = 1.5;
00086     thee->density = 3.0;
00087
00088     thee->setsurf = 0;
00089     thee->surfct = 0;
00090
00091     thee->setimat = 0;
00092     thee->imatct = 0;
00093
00094     thee->setexp = 0;
00095     thee->expct = 0;
00096
00097     return VRC_SUCCESS;
00098 }
00099
00100 VPUBLIC void PBSAMParm_dtor(PBSAMParm **thee) {
00101     if ((*thee) != VNULL) {
00102         PBSAMParm_dtor2(*thee);
00103         Vmem_free(VNULL, 1, sizeof(PBSAMParm), (void **)thee);
00104         (*thee) = VNULL;
00105     }
00106 }
00107
00108 VPUBLIC void PBSAMParm_dtor2(PBSAMParm *thee) { ; }
00109
00110 VPUBLIC Vrc_Codes PBSAMParm_check(PBSAMParm *thee) {
00111
00112     Vrc_Codes rc;
00113
00114     rc = VRC_SUCCESS;
00115
00116     Vnm_print(0, "PBSAMParm_check:  checking PBSAMParm object of type %d.\n",
00117         thee->type);
00118
00119     /* Check to see if we were even filled... */
00120     if (!thee->parsed) {
00121         Vnm_print(2, "PBSAMParm_check:  not filled!\n");

```

```

00122         return VRC_FAILURE;
00123     }
00124
00125     /* Check type settings */
00126     if(thee->type != PBSAMCT_AUTO) {
00127         Vnm_print(2, "PBSAMparm_check: type not set");
00128         rc = VRC_FAILURE;
00129     }
00130
00131     return rc;
00132 }
00133
00134
00135 VPUBLIC void PBSAMparm_copy(PBSAMparm *thee, PBSAMparm *parm) {
00136     int i, j;
00137     VASSERT(thee != VNULL);
00138     VASSERT(parm != VNULL);
00139
00140     thee->settolsp = parm->settolsp;
00141     thee->tolsp = parm->tolsp;
00142
00143     thee->setmsms = parm->setmsms;
00144     thee->probe_radius = parm->probe_radius;
00145     thee->density = parm->density;
00146     thee->setsurf = parm->setsurf;
00147     thee->surfct = parm->surfct;
00148     thee->setimat = parm->setimat;
00149     thee->imatct = parm->imatct;
00150     thee->setexp = parm->setexp;
00151     thee->expct = parm->expct;
00152
00153     for (i=0; i<PBSAMPARM_MAXWRITE; i++)
00154     {
00155         for (j=0; j<CHR_MAXLEN; j++)
00156         {
00157             thee->surffil[i][j] = parm->surffil[i][j];
00158             thee->imatfil[i][j] = parm->imatfil[i][j];
00159             thee->expfil[i][j] = parm->expfil[i][j];
00160         }
00161     }
00162 }
00163
00164 //Parsing vertex file
00165 VPRIVATE Vrc_Codes PBSAMparm_parseSurf(PBSAMparm *thee, Vio *sock){
00166     const char* name = "usemesh";
00167     char tok[VMAX_BUFSIZE];
00168
00169     if(Vio_scanf(sock, "%s", tok) == 0) {
00170         Vnm_print(2, "parsePBSAM: ran out of tokens on %s!\n", name);
00171         return VRC_WARNING;
00172     } else {
00173         strncpy(thee->surffil[thee->surfct], tok, CHR_MAXLEN);
00174         thee->surfct += 1;
00175     }
00176     return VRC_SUCCESS;
00177 }
00178
00179 //Parsing imat prefix file
00180 VPRIVATE Vrc_Codes PBSAMparm_parseMSMS(PBSAMparm *thee, Vio *sock){
00181     int td;
00182     char tok[VMAX_BUFSIZE];
00183     const char *name = "mesh";
00184
00185     if(Vio_scanf(sock, "%s", tok) == 0){
00186         Vnm_print(2, "parsePBSAM: ran out of tokens on %s!\n", name);
00187         return VRC_WARNING;
00188     }
00189     if(strcmp(tok, "msms") == 0){
00190         thee->setmsms = 1;
00191     }
00192     else{
00193         Vnm_print(2, "parsePBSAM: %s is not currently supported in PBSAM! Change to msms\n", tok);
00194         return VRC_WARNING;
00195     }
00196     return VRC_SUCCESS;
00197 }
00198
00199 //Parsing imat prefix file

```

```

00203 VPRIVATE Vrc_Codes PBSAMparm_parseImat(PBSAMparm *thee, Vio *sock){
00204     const char* name = "imat";
00205     char tok[VMAX_BUFSIZE];
00206
00207     if(Vio_scanf(sock, "%s", tok) == 0) {
00208         Vnm_print(2, "parsePBSAM: ran out of tokens on %s!\n", name);
00209         return VRC_WARNING;
00210     } else {
00211         strncpy(thee->imatfil[thee->imatct], tok, CHR_MAXLEN);
00212         thee->imatct += 1;
00213     }
00214     return VRC_SUCCESS;
00215 }
00216
00217 //Parsing imat prefix file
00218 VPRIVATE Vrc_Codes PBSAMparm_parseExp(PBSAMparm *thee, Vio *sock){
00219     const char* name = "exp";
00220     char tok[VMAX_BUFSIZE];
00221
00222     if(Vio_scanf(sock, "%s", tok) == 0) {
00223         Vnm_print(2, "parsePBSAM: ran out of tokens on %s!\n", name);
00224         return VRC_WARNING;
00225     } else {
00226         strncpy(thee->expfil[thee->expct], tok, CHR_MAXLEN);
00227         thee->expct += 1;
00228     }
00229     return VRC_SUCCESS;
00230 }
00231
00232 VPRIVATE Vrc_Codes PBSAMparm_parseTolsp(PBSAMparm *thee, Vio *sock){
00233     const char* name = "tolsp";
00234     char tok[VMAX_BUFSIZE];
00235     double tf;
00236     if(Vio_scanf(sock, "%s", tok) == 0) {
00237         Vnm_print(2, "parsePBSAM: ran out of tokens on %s!\n", name);
00238         return VRC_WARNING;
00239     }
00240
00241     if (sscanf(tok, "%lf", &tf) == 0){
00242         Vnm_print(2, "Nosh: Read non-float (%s) while parsing %s keyword!\n", tok, name);
00243         return VRC_WARNING;
00244     }else{
00245         thee->tolsp = tf;
00246     }
00247     thee->settolsp = 1;
00248     return VRC_SUCCESS;
00249 }
00250
00251
00252 VPUBLIC Vrc_Codes PBSAMparm_parseToken(PBSAMparm *thee, char tok[VMAX_BUFSIZE],
00253     Vio *sock) {
00254
00255     if (thee == VNULL) {
00256         Vnm_print(2, "parsePBSAM: got NULL thee!\n");
00257         return VRC_WARNING;
00258     }
00259     if (sock == VNULL) {
00260         Vnm_print(2, "parsePBSAM: got NULL socket!\n");
00261         return VRC_WARNING;
00262     }
00263
00264     Vnm_print(0, "PBSAMparm_parseToken: trying %s...\n", tok);
00265
00266     // Molecule terms
00267     if (Vstring_strcasecmp(tok, "usemesh") == 0) {
00268         return PBSAMparm_parseSurf(thee, sock);
00269     }else if (Vstring_strcasecmp(tok, "mesh") == 0) {
00270         return PBSAMparm_parseMSMS(thee, sock);
00271     }else if (Vstring_strcasecmp(tok, "imat") == 0) {
00272         return PBSAMparm_parseImat(thee, sock);
00273     }else if (Vstring_strcasecmp(tok, "exp") == 0) {
00274         return PBSAMparm_parseExp(thee, sock);
00275     }else if (Vstring_strcasecmp(tok, "tolsp") == 0) {
00276         return PBSAMparm_parseTolsp(thee, sock);
00277     }
00278
00279     else {
00280         Vnm_print(2, "parsePBSAM: Unrecognized keyword (%s)!\n", tok);
00281         return VRC_WARNING;
00282     }
00283     return VRC_FAILURE;

```

```
00284 }
```

9.48 src/generic/pbsamparm.h File Reference

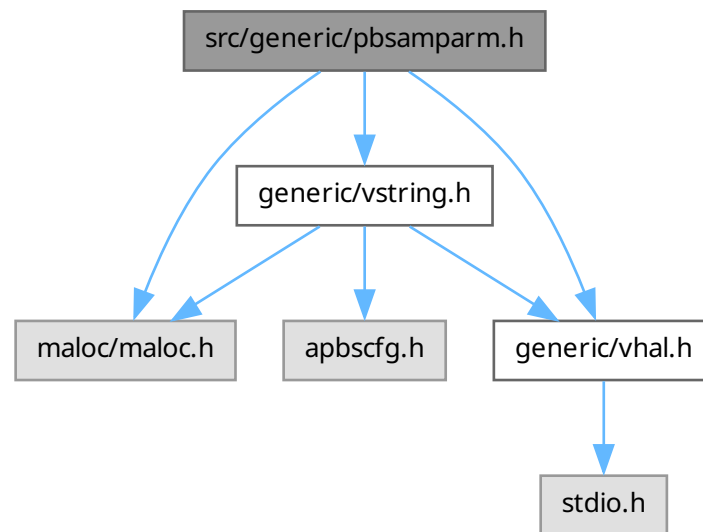
Contains declarations for class PBSAMparm.

```
#include "maloc/maloc.h"
```

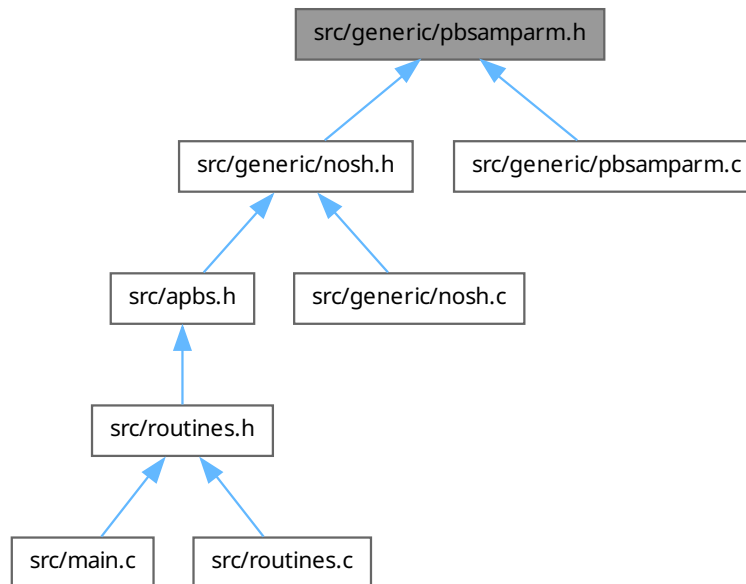
```
#include "generic/vhal.h"
```

```
#include "generic/vstring.h"
```

Include dependency graph for pbsamparm.h:



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [sPBSAMparm](#)
Parameter structure for PBSAM-specific variables from input files.

Macros

- #define [CHR_MAXLEN](#) 1000
Number of things that can be written out in a single calculation.
- #define [PBSAMPARM_MAXWRITE](#) 15
- #define [PBSAMPARM_MAXMOL](#) 150

Typedefs

- typedef enum [ePBSAMparm_CalcType](#) [PBSAMparm_CalcType](#)
Declare PBSAMparm_CalcType type.
- typedef struct [sPBSAMparm](#) [PBSAMparm](#)
Parameter structure for PBSAM-specific variables from input files.

Enumerations

- enum [ePBSAMparm_CalcType](#) { [PBSAMCT_AUTO](#) =1 }
Calculation type.

Functions

- VEXTERNC `PBSAMparm * PBSAMparm_ctor (PBSAMparm_CalcType type)`
Construct PBSAMparm object.
- VEXTERNC `Vrc_Codes PBSAMparm_ctor2 (PBSAMparm *thee, PBSAMparm_CalcType type)`
FORTTRAN stub to construct PBSAMparm object ?????????!!!!!!!
- VEXTERNC `void PBSAMparm_dtor (PBSAMparm **thee)`
Object destructor.
- VEXTERNC `void PBSAMparm_dtor2 (PBSAMparm *thee)`
FORTTRAN stub for object destructor ?????????!!!!!!!
- VEXTERNC `Vrc_Codes PBSAMparm_check (PBSAMparm *thee)`
Consistency check for parameter values stored in object.
- VEXTERNC `Vrc_Codes PBSAMparm_parseToken (PBSAMparm *thee, char tok[VMAX_BUFSIZE], Vio *sock)`
Parse an MG keyword from an input file.
- VEXTERNC `void PBSAMparm_copy (PBSAMparm *thee, PBSAMparm *parm)`
copy PBSAMparm object into thee.
- VPRIVATE `Vrc_Codes PBSAMparm_parseTolsp (PBSAMparm *thee, Vio *sock)`
Find sphere tolerance for coarse-graining.
- VPRIVATE `Vrc_Codes PBSAMparm_parseSurf (PBSAMparm *thee, Vio *sock)`
Find vertex files for each molecule and save them.
- VPRIVATE `Vrc_Codes PBSAMparm_parselmat (PBSAMparm *thee, Vio *sock)`
Find IMAT files for each molecule and save them.
- VPRIVATE `Vrc_Codes PBSAMparm_parseExp (PBSAMparm *thee, Vio *sock)`
Find expansion files for each molecule and save them.
- VPRIVATE `Vrc_Codes PBSAMparm_parseMSMS (PBSAMparm *thee, Vio *sock)`
Find msms flag for if MSMS is to be run.

9.48.1 Detailed Description

Contains declarations for class PBSAMparm.

Version

\$Id\$

Author

Lisa Felberg

Attention

```
*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
* Nathan A. Baker (nathan.baker@pnnl.gov)
* Pacific Northwest National Laboratory
*
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*
*

```

Definition in file [pbsamparm.h](#).

9.48.2 Macro Definition Documentation

9.48.2.1 PBSAMPARM_MAXMOL

```
#define PBSAMPARM_MAXMOL 150
```

Definition at line 78 of file [pbsamparm.h](#).

9.48.2.2 PBSAMPARM_MAXWRITE

```
#define PBSAMPARM_MAXWRITE 15
```

Definition at line 77 of file [pbsamparm.h](#).

9.49 pbsamparm.h

[Go to the documentation of this file.](#)

```

00001
00064 #ifndef _PBSAMPARM_H_
00065 #define _PBSAMPARM_H_
00066
00067 /* Generic header files */
00068 #include "malloc/malloc.h"
00069
00070 #include "generic/vhal.h"
00071 #include "generic/vstring.h"
00072
00076 #define CHR_MAXLEN 1000
00077 #define PBSAMPARM_MAXWRITE 15
00078 #define PBSAMPARM_MAXMOL 150
00079
00084 enum ePBSAMparm_CalcType {
00085     //other methods disabled for now only auto currently implemented.

```

```

00086 //PBSAMCT_MANUAL=0, /**< PBSAM-manual */
00087     PBSAMCT_AUTO=1,
00088     //PBSAMCT_NONE=2 /**< not defined */
00089 };
00090
00095 typedef enum ePBSAmparm_CalcType PBSAmparm_CalcType;
00096
00105 typedef struct sPBSAmparm {
00106
00107     PBSAmparm_CalcType type;
00108     int parsed;
00110     /* The only parms in addition to PBAM would be MSMS
00111        IMAT and Selfpol */
00112     int settolsp;
00113     double tols;
00114
00115     int setmsms;
00116     double probe_radius;
00117     double density;
00118
00119     int setsurf;
00120     int surfct;
00121     char surfhil[PBSAMPARM_MAXMOL][CHR_MAXLEN];
00122
00123     int setimat;
00124     int imatct;
00125     char imatfil[PBSAMPARM_MAXMOL][CHR_MAXLEN];
00126
00127     int setexp;
00128     int expct;
00129     char expfil[PBSAMPARM_MAXMOL][CHR_MAXLEN];
00130
00131 } PBSAmparm;
00132
00139 VEXTERNC PBSAmparm* PBSAmparm_ctor(PBSAmparm_CalcType type);
00140
00148 VEXTERNC Vrc_Codes PBSAmparm_ctor2(PBSAmparm *thee, PBSAmparm_CalcType type);
00149
00155 VEXTERNC void PBSAmparm_dtor(PBSAmparm **thee);
00156
00162 VEXTERNC void PBSAmparm_dtor2(PBSAmparm *thee);
00163
00170 VEXTERNC Vrc_Codes PBSAmparm_check(PBSAmparm *thee);
00171
00181 VEXTERNC Vrc_Codes PBSAmparm_parseToken(PBSAmparm *thee, char tok[VMAX_BUFSIZE],
00182     Vio *sock);
00190 VEXTERNC void PBSAmparm_copy(PBSAmparm *thee, PBSAmparm *parm);
00191
00199 VPRIVATE Vrc_Codes PBSAmparm_parseTolsp(PBSAmparm *thee, Vio *sock);
00200
00208 VPRIVATE Vrc_Codes PBSAmparm_parseSurf(PBSAmparm *thee, Vio *sock);
00209
00217 VPRIVATE Vrc_Codes PBSAmparm_parseImat(PBSAmparm *thee, Vio *sock);
00218
00226 VPRIVATE Vrc_Codes PBSAmparm_parseExp(PBSAmparm *thee, Vio *sock);
00227
00235 VPRIVATE Vrc_Codes PBSAmparm_parseMSMS(PBSAmparm *thee, Vio *sock);
00236
00237 #endif
00238

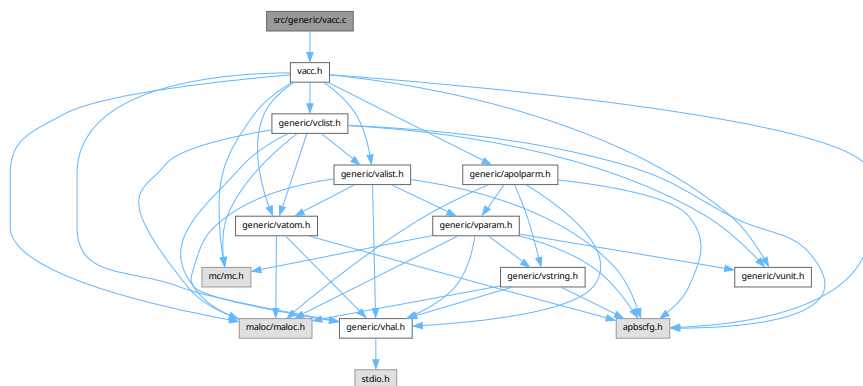
```

9.50 src/generic/vacc.c File Reference

Class Vacc methods.

```
#include "vacc.h"
```

Include dependency graph for vacc.c:



Functions

- VPUBLIC unsigned long int [Vacc_memChk](#) ([Vacc](#) *three)
Get number of bytes in this object and its members.
- VPRIVATE int [ivdwAccExclus](#) ([Vacc](#) *three, double center[3], double radius, int atomID)
Determines if a point is within the union of the spheres centered at the atomic centers with radii equal to the sum of their van der Waals radii and the probe radius. Does not include contributions from the specified atom.
- VPUBLIC [Vacc](#) * [Vacc_ctor](#) ([Valist](#) *alist, [Vclist](#) *clist, double surf_density)
Construct the accessibility object.
- VPRIVATE int [Vacc_storeParms](#) ([Vacc](#) *three, [Valist](#) *alist, [Vclist](#) *clist, double surf_density)
- VPRIVATE int [Vacc_allocate](#) ([Vacc](#) *three)
- VPUBLIC int [Vacc_ctor2](#) ([Vacc](#) *three, [Valist](#) *alist, [Vclist](#) *clist, double surf_density)
FORTTRAN stub to construct the accessibility object.
- VPUBLIC void [Vacc_dtor](#) ([Vacc](#) **three)
Destroy object.
- VPUBLIC void [Vacc_dtor2](#) ([Vacc](#) *three)
FORTTRAN stub to destroy object.
- VPUBLIC double [Vacc_vdwAcc](#) ([Vacc](#) *three, double center[3])
- VPUBLIC double [Vacc_ivdwAcc](#) ([Vacc](#) *three, double center[3], double radius)
- VPUBLIC void [Vacc_splineAccGradAtomNorm](#) ([Vacc](#) *three, double center[VAPBS_DIM], double win, double infrad, [Vatom](#) *atom, double *grad)
Report gradient of spline-based accessibility with respect to a particular atom normalized by the accessibility value due to that atom at that point (see [Vpmg_splineAccAtom](#))
- VPUBLIC void [Vacc_splineAccGradAtomUnnorm](#) ([Vacc](#) *three, double center[VAPBS_DIM], double win, double infrad, [Vatom](#) *atom, double *grad)
Report gradient of spline-based accessibility with respect to a particular atom (see [Vpmg_splineAccAtom](#))
- VPUBLIC double [Vacc_splineAccAtom](#) ([Vacc](#) *three, double center[VAPBS_DIM], double win, double infrad, [Vatom](#) *atom)
Report spline-based accessibility for a given atom.
- VPRIVATE double [splineAcc](#) ([Vacc](#) *three, double center[VAPBS_DIM], double win, double infrad, [VclistCell](#) *cell)
Fast spline-based surface computation subroutine.
- VPUBLIC double [Vacc_splineAcc](#) ([Vacc](#) *three, double center[VAPBS_DIM], double win, double infrad)

Report spline-based accessibility.

- VPUBLIC void `Vacc_splineAccGrad` (`Vacc` *thee, double center[`VAPBS_DIM`], double win, double infrad, double *grad)

Report gradient of spline-based accessibility.

- VPUBLIC double `Vacc_molAcc` (`Vacc` *thee, double center[`VAPBS_DIM`], double radius)

Report molecular accessibility.

- VPUBLIC double `Vacc_fastMolAcc` (`Vacc` *thee, double center[`VAPBS_DIM`], double radius)

Report molecular accessibility quickly.

- VPUBLIC void `Vacc_writeGMV` (`Vacc` *thee, double radius, int meth, Gem *gm, char *iodev, char *iofmt, char *iohost, char *iofile)
- VPUBLIC double `Vacc_SASA` (`Vacc` *thee, double radius)

Build the solvent accessible surface (SAS) and calculate the solvent accessible surface area.

- VPUBLIC double `Vacc_totalSASA` (`Vacc` *thee, double radius)

Return the total solvent accessible surface area (SASA)

- VPUBLIC double `Vacc_atomSASA` (`Vacc` *thee, double radius, `Vatom` *atom)

Return the atomic solvent accessible surface area (SASA)

- VPUBLIC `VaccSurf` * `VaccSurf_ctor` (`Vmem` *mem, double probe_radius, int nsphere)

Allocate and construct the surface object; do not assign surface points to positions.

- VPUBLIC int `VaccSurf_ctor2` (`VaccSurf` *thee, `Vmem` *mem, double probe_radius, int nsphere)

Construct the surface object using previously allocated memory; do not assign surface points to positions.

- VPUBLIC void `VaccSurf_dtor` (`VaccSurf` **thee)

Destroy the surface object and free its memory.

- VPUBLIC void `VaccSurf_dtor2` (`VaccSurf` *thee)

Destroy the surface object.

- VPUBLIC `VaccSurf` * `Vacc_atomSurf` (`Vacc` *thee, `Vatom` *atom, `VaccSurf` *ref, double prad)

Set up an array of points corresponding to the SAS due to a particular atom.

- VPUBLIC `VaccSurf` * `VaccSurf_refSphere` (`Vmem` *mem, int npts)

Set up an array of points for a reference sphere of unit radius.

- VPUBLIC `VaccSurf` * `Vacc_atomSASPoints` (`Vacc` *thee, double radius, `Vatom` *atom)

Get the set of points for this atom's solvent-accessible surface.

- VPUBLIC void `Vacc_splineAccGradAtomNorm4` (`Vacc` *thee, double center[`VAPBS_DIM`], double win, double infrad, `Vatom` *atom, double *grad)

Report gradient of spline-based accessibility with respect to a particular atom normalized by a 4th order accessibility value due to that atom at that point (see `Vpmsg_splineAccAtom`)

- VPUBLIC void `Vacc_splineAccGradAtomNorm3` (`Vacc` *thee, double center[`VAPBS_DIM`], double win, double infrad, `Vatom` *atom, double *grad)

Report gradient of spline-based accessibility with respect to a particular atom normalized by a 3rd order accessibility value due to that atom at that point (see `Vpmsg_splineAccAtom`)

- VPUBLIC void `Vacc_atomdSAV` (`Vacc` *thee, double srاد, `Vatom` *atom, double *dSA)

Get the derivatve of solvent accessible volume.

- VPRIVATE double `Vacc_SASAPos` (`Vacc` *thee, double radius)
- VPRIVATE double `Vacc_atomSASAPos` (`Vacc` *thee, double radius, `Vatom` *atom, int mode)
- VPUBLIC void `Vacc_atomdSASA` (`Vacc` *thee, double dpos, double srاد, `Vatom` *atom, double *dSA)

Get the derivatve of solvent accessible area.

- VPUBLIC void `Vacc_totalAtomdSASA` (`Vacc` *thee, double dpos, double srاد, `Vatom` *atom, double *dSA)

Testing purposes only.

- VPUBLIC void `Vacc_totalAtomdSAV` (`Vacc` *thee, double dpos, double srاد, `Vatom` *atom, double *dSA, `Vclist` *clist)

Total solvent accessible volume.

- VPUBLIC double [Vacc_totalSAV](#) ([Vacc](#) *thee, [Vclist](#) *clist, [APOLparm](#) *apolparm, double radius)

Return the total solvent accessible volume (SAV)

- int [Vacc_wcaEnergyAtom](#) ([Vacc](#) *thee, [APOLparm](#) *apolparm, [Valist](#) *alist, [Vclist](#) *clist, int iatom, double *value)

Calculate the WCA energy for an atom.

- VPUBLIC int [Vacc_wcaEnergy](#) ([Vacc](#) *acc, [APOLparm](#) *apolparm, [Valist](#) *alist, [Vclist](#) *clist)

Return the WCA integral energy.

- VPUBLIC int [Vacc_wcaForceAtom](#) ([Vacc](#) *thee, [APOLparm](#) *apolparm, [Vclist](#) *clist, [Vatom](#) *atom, double *force)

Return the WCA integral force.

9.50.1 Detailed Description

Class Vacc methods.

Author

Nathan Baker

Version

\$Id\$

Attention

```
*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
* Nathan A. Baker (nathan.baker@pnnl.gov)
* Pacific Northwest National Laboratory
*
* Additional contributing authors listed in the code documentation.
*
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```

```

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* THE POSSIBILITY OF SUCH DAMAGE.
*
*

```

Definition in file [vacc.c](#).

9.50.2 Function Documentation

9.50.2.1 ivdwAccExclus()

```

VPRIVATE int ivdwAccExclus (
    Vacc * thee,
    double center[3],
    double radius,
    int atomID )

```

Determines if a point is within the union of the spheres centered at the atomic centers with radii equal to the sum of their van der Waals radii and the probe radius. Does not include contributions from the specified atom.

Returns

1 if accessible (outside the inflated van der Waals radius), 0 otherwise

Author

Nathan Baker

Parameters

<i>center</i>	Accessibility object
<i>radius</i>	Position to test
<i>atomID</i>	Radius of probe ID of atom to ignore

Definition at line 80 of file [vacc.c](#).

9.50.2.2 splineAcc()

```

VPRIVATE double splineAcc (
    Vacc * thee,
    double center[VAPBS_DIM],
    double win,
    double infrad,
    VclistCell * cell )

```

Fast spline-based surface computation subroutine.

Returns

Spline value

Author

Todd Dolinsky and Nathan Baker

Parameters

<i>center</i>	Accessibility object
<i>win</i>	Point at which the acc is to be evaluated
<i>infrad</i>	Spline window
<i>cell</i>	Radius to inflate atomic radius Cell of atom objects

Definition at line 493 of file [vacc.c](#).

9.50.2.3 Vacc_allocate()

```
VPRIVATE int Vacc_allocate (
    Vacc * thee )
```

Allocate (and clear) space for storage

Definition at line 193 of file [vacc.c](#).

9.50.2.4 Vacc_atomSASAPos()

```
VPRIVATE double Vacc_atomSASAPos (
    Vacc * thee,
    double radius,
    Vatom * atom,
    int mode )
```

Definition at line 1277 of file [vacc.c](#).

9.50.2.5 Vacc_ivdwAcc()

```
VPUBLIC double Vacc_ivdwAcc (
    Vacc * thee,
    double center[3],
    double radius )
```

Definition at line 307 of file [vacc.c](#).

9.50.2.6 Vacc_SASAPos()

```
VPRIVATE double Vacc_SASAPos (
    Vacc * thee,
    double radius )
```

Definition at line 1252 of file [vacc.c](#).

9.50.2.7 Vacc_storeParms()

```
VPRIVATE int Vacc_storeParms (
    Vacc * thee,
    Valist * alist,
    Vclist * clist,
    double surf_density )
```

Check and store parameters passed to constructor

Definition at line 148 of file [vacc.c](#).

9.50.2.8 Vacc_vdwAcc()

```
VPUBLIC double Vacc_vdwAcc (
    Vacc * thee,
    double center[3] )
```

Definition at line 277 of file [vacc.c](#).

9.50.2.9 Vacc_writeGMV()

```
VPUBLIC void Vacc_writeGMV (
    Vacc * thee,
    double radius,
    int meth,
    Gem * gm,
    char * iodev,
    char * iofmt,
    char * iohost,
    char * iofile )
```

Definition at line 679 of file [vacc.c](#).

9.51 vacc.c

[Go to the documentation of this file.](#)

```
00001
00057 #include "vacc.h"
00058
00059 VEMBED(rcsid="$Id$")
00060
00061 #if !defined(VINLINE_VACC)
00062
00063 VPUBLIC unsigned long int Vacc_memChk(Vacc *thee) {
00064     if (thee == VNULL)
00065         return 0;
00066     return Vmem_bytes(thee->mem);
00067 }
00068
00069 #endif /* if !defined(VINLINE_VACC) */
00070
00080 VPRIVATE int ivdwAccExclus(
00081     Vacc *thee,
00082     double center[3],
00083     double radius,
00084     int atomID
00085 ) {
00086
00087     int iatom;
00088     double dist2,
00089         *apos;
00090     Vatom *atom;
00091     VclistCell *cell;
00092
00093     VASSERT(thee != VNULL);
00094
00095     /* We can only test probes with radii less than the max specified */
00096     if (radius > Vclist_maxRadius(thee->clist)) {
00097         Vnm_print(2,
00098             "Vacc_ivdwAcc: got radius (%g) bigger than max radius (%g)\n",
00099             radius, Vclist_maxRadius(thee->clist));
00100         VASSERT(0);
00101     }
00102
00103     /* Get the relevant cell from the cell list */
00104     cell = Vclist_getCell(thee->clist, center);
00105
00106     /* If we have no cell, then no atoms are nearby and we're definitely
00107      * accessible */
00108     if (cell == VNULL) {
00109         return 1;
00110     }
00111
00112     /* Otherwise, check for overlap with the atoms in the cell */
00113     for (iatom=0; iatom<cell->natoms; iatom++) {
00114         atom = cell->atoms[iatom];
00115
00116         // We don't actually need to test this if the atom IDs do match; don't compute this if we're
00117         // comparing atom against itself.
00117         if (atom->id == atomID) continue;
```

```

00118
00119     apos = atom->position;
00120     dist2 = VSQR(center[0]-apos[0]) + VSQR(center[1]-apos[1])
00121           + VSQR(center[2]-apos[2]);
00122     if (dist2 < VSQR(atom->radius+radius)){
00123         return 0;
00124     }
00125 }
00126
00127 /* If we're still here, then the point is accessible */
00128 return 1;
00129
00130 }
00131
00132 VPUBLIC Vacc* Vacc_ctor(Valist *alist,
00133                         Vclist *clist,
00134                         double surf_density /* Surface density */
00135                         ) {
00136
00137     Vacc *thee = VNULL;
00138
00139     /* Set up the structure */
00140     thee = (Vacc*)Vmem_malloc(VNULL, 1, sizeof(Vacc) );
00141     VASSERT( thee != VNULL);
00142     VASSERT( Vacc_ctor2(thee, alist, clist, surf_density));
00143     return thee;
00144 }
00145
00146
00147 VPRIVATE int Vacc_storeParms(Vacc *thee,
00148                             Valist *alist,
00149                             Vclist *clist,
00150                             double surf_density /* Surface density */
00151                             ) {
00152
00153     int nsphere,
00154         iatom;
00155     double maxrad = 0.0,
00156         maxarea,
00157         rad;
00158     Vatom *atom;
00159
00160     if (alist == VNULL) {
00161         Vnm_print(2, "Vacc_storeParms: Got NULL Valist!\n");
00162         return 0;
00163     } else thee->alist = alist;
00164     if (clist == VNULL) {
00165         Vnm_print(2, "Vacc_storeParms: Got NULL Vclist!\n");
00166         return 0;
00167     } else thee->clist = clist;
00168     thee->surf_density = surf_density;
00169
00170     /* Loop through the atoms to determine the maximum radius */
00171     maxrad = 0.0;
00172     for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
00173         atom = Valist_getAtom(alist, iatom);
00174         rad = Vatom_getRadius(atom);
00175         if (rad > maxrad) maxrad = rad;
00176     }
00177     maxrad = maxrad + Vclist_maxRadius(thee->clist);
00178
00179     maxarea = 4.0*VPI*maxrad*maxrad;
00180     nsphere = (int)ceil(maxarea*surf_density);
00181
00182     Vnm_print(0, "Vacc_storeParms: Surf. density = %g\n", surf_density);
00183     Vnm_print(0, "Vacc_storeParms: Max area = %g\n", maxarea);
00184     thee->refSphere = VaccSurf_refSphere(thee->mem, nsphere);
00185     Vnm_print(0, "Vacc_storeParms: Using %d-point reference sphere\n",
00186             thee->refSphere->npts);
00187
00188     return 1;
00189 }
00190
00191
00192 VPRIVATE int Vacc_allocate(Vacc *thee) {
00193
00194     int i,
00195         natoms;
00196
00197     natoms = Valist_getNumberAtoms(thee->alist);
00198
00199     thee->atomFlags = (int*)Vmem_malloc(thee->mem, natoms, sizeof(int));
00200

```

```

00201     if (thee->atomFlags == VNULL) {
00202         Vnm_print(2,
00203             "Vacc_allocate: Failed to allocate %d (int)s for atomFlags!\n",
00204             natoms);
00205         return 0;
00206     }
00207     for (i=0; i<natoms; i++) (thee->atomFlags)[i] = 0;
00208
00209     return 1;
00210 }
00211
00212
00213 VPUBLIC int Vacc_ctor2(Vacc *thee,
00214                     Valist *alist,
00215                     Vclist *clist,
00216                     double surf_density
00217                     ) {
00218
00219     /* Check and store parameters */
00220     if (!Vacc_storeParms(thee, alist, clist, surf_density)) {
00221         Vnm_print(2, "Vacc_ctor2: parameter check failed!\n");
00222         return 0;
00223     }
00224
00225     /* Set up memory management object */
00226     thee->mem = Vmem_ctor("APBS::VACC");
00227     if (thee->mem == VNULL) {
00228         Vnm_print(2, "Vacc_ctor2: memory object setup failed!\n");
00229         return 0;
00230     }
00231
00232     /* Setup and check probe */
00233     thee->surf = VNULL;
00234
00235     /* Allocate space */
00236     if (!Vacc_allocate(thee)) {
00237         Vnm_print(2, "Vacc_ctor2: memory allocation failed!\n");
00238         return 0;
00239     }
00240
00241     return 1;
00242 }
00243
00244
00245 VPUBLIC void Vacc_dtor(Vacc **thee) {
00246
00247     if ((*thee) != VNULL) {
00248         Vacc_dtor2(*thee);
00249         Vmem_free(VNULL, 1, sizeof(Vacc), (void **)thee);
00250         (*thee) = VNULL;
00251     }
00252
00253 }
00254
00255 VPUBLIC void Vacc_dtor2(Vacc *thee) {
00256
00257     int i,
00258         natoms;
00259
00260     natoms = Valist_getNumberAtoms(thee->alist);
00261     Vmem_free(thee->mem, natoms, sizeof(int), (void **)&(thee->atomFlags));
00262
00263     if (thee->refSphere != VNULL) {
00264         VaccSurf_dtor(&(thee->refSphere));
00265         thee->refSphere = VNULL;
00266     }
00267     if (thee->surf != VNULL) {
00268         for (i=0; i<natoms; i++) VaccSurf_dtor(&(thee->surf[i]));
00269         Vmem_free(thee->mem, natoms, sizeof(VaccSurf *),
00270             (void **)&(thee->surf));
00271         thee->surf = VNULL;
00272     }
00273
00274     Vmem_dtor(&(thee->mem));
00275 }
00276
00277 VPUBLIC double Vacc_vdwAcc(Vacc *thee,
00278                         double center[3]
00279                         ) {
00280
00281     VclistCell *cell;

```

```

00282     Vatom *atom;
00283     int iatom;
00284     double *apos,
00285           dist2;
00286
00287     /* Get the relevant cell from the cell list */
00288     cell = Vclist_getCell(thee->clist, center);
00289
00290     /* If we have no cell, then no atoms are nearby and we're definitely
00291      * accessible */
00292     if (cell == VNULL) return 1.0;
00293
00294     /* Otherwise, check for overlap with the atoms in the cell */
00295     for (iatom=0; iatom<cell->natoms; iatom++) {
00296         atom = cell->atoms[iatom];
00297         apos = Vatom_getPosition(atom);
00298         dist2 = VSQR(center[0]-apos[0]) + VSQR(center[1]-apos[1])
00299               + VSQR(center[2]-apos[2]);
00300         if (dist2 < VSQR(Vatom_getRadius(atom))) return 0.0;
00301     }
00302
00303     /* If we're still here, then the point is accessible */
00304     return 1.0;
00305 }
00306
00307 VPUBLIC double Vacc_ivdwAcc(Vacc *thee,
00308                           double center[3],
00309                           double radius
00310                           ) {
00311
00312     return (double)ivdwAccExclus(thee, center, radius, -1);
00313 }
00314 }
00315
00316 VPUBLIC void Vacc_splineAccGradAtomNorm(Vacc *thee,
00317                                         double center[VAPBS_DIM],
00318                                         double win,
00319                                         double infrad,
00320                                         Vatom *atom,
00321                                         double *grad
00322                                         ) {
00323
00324     int i;
00325     double dist,
00326           *apos,
00327           arad,
00328           sm,
00329           sm2,
00330           w2i, /* inverse of win squared */
00331           w3i, /* inverse of win cubed */
00332           mygrad,
00333           mychi = 1.0; /* Char. func. value for given atom */
00334
00335     VASSERT(thee != NULL);
00336
00337     /* Inverse squared window parameter */
00338     w2i = 1.0/(win*win);
00339     w3i = 1.0/(win*win*win);
00340
00341     /* The grad is zero by default */
00342     for (i=0; i<VAPBS_DIM; i++) grad[i] = 0.0;
00343
00344     /* *** CALCULATE THE CHARACTERISTIC FUNCTION VALUE FOR THIS ATOM AND THE
00345      * *** MAGNITUDE OF THE FORCE *** */
00346     apos = Vatom_getPosition(atom);
00347     /* Zero-radius atoms don't contribute */
00348     if (Vatom_getRadius(atom) > 0.0) {
00349         arad = Vatom_getRadius(atom) + infrad;
00350         dist = VSQR(VSQR(apos[0]-center[0]) + VSQR(apos[1]-center[1])
00351               + VSQR(apos[2]-center[2]));
00352         /* If we're inside an atom, the entire characteristic function
00353          * will be zero and the grad will be zero, so we can stop */
00354         if (dist < (arad - win)) return;
00355         /* Likewise, if we're outside the smoothing window, the characteristic
00356          * function is unity and the grad will be zero, so we can stop */
00357         else if (dist > (arad + win)) return;
00358         /* Account for floating point error at the border
00359          * NAB: COULDN'T THESE TESTS BE COMBINED AS BELOW
00360          * (Vacc_splineAccAtom)? */
00361         else if ((VABS(dist - (arad - win)) < VSMALL) ||
00362                  (VABS(dist - (arad + win)) < VSMALL)) return;

```

```

00363     /* If we're inside the smoothing window */
00364     else {
00365         sm = dist - arad + win;
00366         sm2 = VSQR(sm);
00367         mychi = 0.75*sm2*w2i - 0.25*sm*sm2*w3i;
00368         mygrad = 1.5*sm*w2i - 0.75*sm2*w3i;
00369     }
00370     /* Now assemble the grad vector */
00371     VASSERT(mychi > 0.0);
00372     for (i=0; i<VAPBS_DIM; i++)
00373         grad[i] = -(mygrad/mychi)*((center[i] - apos[i])/dist);
00374 }
00375 }
00376
00377 VPUBLIC void Vacc_splineAccGradAtomUnnorm(Vacc *thee,
00378     double center[VAPBS_DIM],
00379     double win,
00380     double infrad,
00381     Vatom *atom,
00382     double *grad
00383 ) {
00384
00385     int i;
00386     double dist,
00387         *apos,
00388         arad,
00389         sm,
00390         sm2,
00391         w2i, /* Inverse of win squared */
00392         w3i, /* Inverse of win cubed */
00393         mygrad,
00394         mychi = 1.0; /* Char. func. value for given atom */
00395
00396     VASSERT(thee != NULL);
00397
00398     /* Inverse squared window parameter */
00399     w2i = 1.0/(win*win);
00400     w3i = 1.0/(win*win*win);
00401
00402     /* The grad is zero by default */
00403     for (i=0; i<VAPBS_DIM; i++) grad[i] = 0.0;
00404
00405     /* *** CALCULATE THE CHARACTERISTIC FUNCTION VALUE FOR THIS ATOM AND THE
00406      * *** MAGNITUDE OF THE FORCE *** */
00407     apos = Vatom_getPosition(atom);
00408     /* Zero-radius atoms don't contribute */
00409     if (Vatom_getRadius(atom) > 0.0) {
00410         arad = Vatom_getRadius(atom) + infrad;
00411         dist = VSQRT(VSQR(apos[0]-center[0]) + VSQR(apos[1]-center[1])
00412             + VSQR(apos[2]-center[2]));
00413         /* If we're inside an atom, the entire characteristic function
00414          * will be zero and the grad will be zero, so we can stop */
00415         if (dist < (arad - win)) return;
00416         /* Likewise, if we're outside the smoothing window, the characteristic
00417          * function is unity and the grad will be zero, so we can stop */
00418         else if (dist > (arad + win)) return;
00419         /* Account for floating point error at the border
00420          * NAB: COULDN'T THESE TESTS BE COMBINED AS BELOW
00421          * (Vacc_splineAccAtom)? */
00422         else if ((VABS(dist - (arad - win)) < VSMALL) ||
00423             (VABS(dist - (arad + win)) < VSMALL)) return;
00424         /* If we're inside the smoothing window */
00425         else {
00426             sm = dist - arad + win;
00427             sm2 = VSQR(sm);
00428             mychi = 0.75*sm2*w2i - 0.25*sm*sm2*w3i;
00429             mygrad = 1.5*sm*w2i - 0.75*sm2*w3i;
00430         }
00431         /* Now assemble the grad vector */
00432         VASSERT(mychi > 0.0);
00433         for (i=0; i<VAPBS_DIM; i++)
00434             grad[i] = -(mygrad)*((center[i] - apos[i])/dist);
00435     }
00436 }
00437
00438 VPUBLIC double Vacc_splineAccAtom(Vacc *thee,
00439     double center[VAPBS_DIM],
00440     double win,
00441     double infrad,
00442     Vatom *atom
00443 ) {

```

```

00444
00445     double dist,
00446         *apos,
00447         arad,
00448         sm,
00449         sm2,
00450         w2i, /* Inverse of win squared */
00451         w3i, /* Inverse of win cubed */
00452         value,
00453         stot,
00454         sctot;
00455
00456     VASSERT(thee != NULL);
00457
00458     /* Inverse squared window parameter */
00459     w2i = 1.0/(win*win);
00460     w3i = 1.0/(win*win*win);
00461
00462     apos = Vatom_getPosition(atom);
00463     /* Zero-radius atoms don't contribute */
00464     if (Vatom_getRadius(atom) > 0.0) {
00465         arad = Vatom_getRadius(atom) + infrad;
00466         stot = arad + win;
00467         sctot = VMAX2(0, (arad - win));
00468         dist = VSQR(VSQR(apos[0]-center[0]) + VSQR(apos[1]-center[1])
00469             + VSQR(apos[2]-center[2]));
00470         /* If we're inside an atom, the entire characteristic function
00471          * will be zero */
00472         if ((dist < sctot) || (VABS(dist - sctot) < VSMALL)){
00473             value = 0.0;
00474             /* We're outside the smoothing window */
00475         } else if ((dist > stot) || (VABS(dist - stot) < VSMALL)) {
00476             value = 1.0;
00477             /* We're inside the smoothing window */
00478         } else {
00479             sm = dist - arad + win;
00480             sm2 = VSQR(sm);
00481             value = 0.75*sm2*w2i - 0.25*sm*sm2*w3i;
00482         }
00483     } else value = 1.0;
00484
00485     return value;
00486 }
00487
00493 VPRIVATE double splineAcc(
00494     Vacc *thee,
00495     double center[VAPBS_DIM],
00496     double win,
00497     double infrad,
00498     VclistCell *cell
00499 ) {
00500
00501     int atomID, iatom;
00502     Vatom *atom;
00503     double value = 1.0;
00504
00505     VASSERT(thee != NULL);
00506
00507     /* Now loop through the atoms assembling the characteristic function */
00508     for (iatom=0; iatom<cell->natoms; iatom++) {
00509
00510         atom = cell->atoms[iatom];
00511         atomID = atom->id;
00512
00513         /* Check to see if we've counted this atom already */
00514         if ( !(thee->atomFlags[atomID]) ) {
00515
00516             thee->atomFlags[atomID] = 1;
00517             value *= Vacc_splineAccAtom(thee, center, win, infrad, atom);
00518
00519             if (value < VSMALL) return value;
00520         }
00521     }
00522
00523     return value;
00524 }
00525
00526
00527
00528 VPUBLIC double Vacc_splineAcc(Vacc *thee, double center[VAPBS_DIM], double win,
00529     double infrad) {
00530

```

```

00531     VclistCell *cell;
00532     Vatom *atom;
00533     int iatom, atomID;
00534
00535
00536     VASSERT(thee != NULL);
00537
00538     if (Vclist_maxRadius(thee->clist) < (win + infrad)) {
00539         Vnm_print(2, "Vacc_splineAcc: Vclist has max_radius=%g;\n",
00540                 Vclist_maxRadius(thee->clist));
00541         Vnm_print(2, "Vacc_splineAcc: Insufficient for win=%g, infrad=%g\n",
00542                 win, infrad);
00543         VASSERT(0);
00544     }
00545
00546     /* Get a cell or VNULL; in the latter case return 1.0 */
00547     cell = Vclist_getCell(thee->clist, center);
00548     if (cell == VNULL) return 1.0;
00549
00550     /* First, reset the list of atom flags
00551      * NAB: THIS SEEMS VERY INEFFICIENT */
00552     for (iatom=0; iatom<cell->natoms; iatom++) {
00553         atom = cell->atoms[iatom];
00554         atomID = atom->id;
00555         thee->atomFlags[atomID] = 0;
00556     }
00557
00558     return splineAcc(thee, center, win, infrad, cell);
00559 }
00560
00561 VPUBLIC void Vacc_splineAccGrad(Vacc *thee, double center[VAPBS_DIM],
00562     double win, double infrad, double *grad) {
00563
00564     int iatom, i, atomID;
00565     double acc = 1.0;
00566     double tgrad[VAPBS_DIM];
00567     VclistCell *cell;
00568     Vatom *atom = VNULL;
00569
00570     VASSERT(thee != NULL);
00571
00572     if (Vclist_maxRadius(thee->clist) < (win + infrad)) {
00573         Vnm_print(2, "Vacc_splineAccGrad: Vclist max_radius=%g;\n",
00574                 Vclist_maxRadius(thee->clist));
00575         Vnm_print(2, "Vacc_splineAccGrad: Insufficient for win=%g, infrad=%g\n",
00576                 win, infrad);
00577         VASSERT(0);
00578     }
00579
00580     /* Reset the gradient */
00581     for (i=0; i<VAPBS_DIM; i++) grad[i] = 0.0;
00582
00583     /* Get the cell; check for nullity */
00584     cell = Vclist_getCell(thee->clist, center);
00585     if (cell == VNULL) return;
00586
00587     /* Reset the list of atom flags */
00588     for (iatom=0; iatom<cell->natoms; iatom++) {
00589         atom = cell->atoms[iatom];
00590         atomID = atom->id;
00591         thee->atomFlags[atomID] = 0;
00592     }
00593
00594     /* Get the local accessibility */
00595     acc = splineAcc(thee, center, win, infrad, cell);
00596
00597     /* Accumulate the gradient of all local atoms */
00598     if (acc > VSMALL) {
00599         for (iatom=0; iatom<cell->natoms; iatom++) {
00600             atom = cell->atoms[iatom];
00601             Vacc_splineAccGradAtomNorm(thee, center, win, infrad, atom, tgrad);
00602         }
00603         for (i=0; i<VAPBS_DIM; i++) grad[i] += tgrad[i];
00604     }
00605     for (i=0; i<VAPBS_DIM; i++) grad[i] *= -acc;
00606 }
00607
00608 VPUBLIC double Vacc_molAcc(Vacc *thee, double center[VAPBS_DIM],
00609     double radius) {
00610
00611     double rc;

```



```

00612
00613 /* ***** CHECK IF OUTSIDE ATOM+PROBE RADIUS SURFACE ***** */
00614 if (Vacc_ivdwAcc(thee, center, radius) == 1.0) {
00615     /* Vnm_print(2, "DEBUG: ivdwAcc = 1.0\n"); */
00616     rc = 1.0;
00617
00618 /* ***** CHECK IF INSIDE ATOM RADIUS SURFACE ***** */
00619 } else if (Vacc_vdwAcc(thee, center) == 0.0) {
00620     /* Vnm_print(2, "DEBUG: vdwAcc = 0.0\n"); */
00621     rc = 0.0;
00622
00623 /* ***** CHECK IF OUTSIDE MOLECULAR SURFACE ***** */
00624 } else {
00625     /* Vnm_print(2, "DEBUG: calling fastMolAcc...\n"); */
00626     rc = Vacc_fastMolAcc(thee, center, radius);
00627 }
00628
00629 return rc;
00630 }
00631
00632
00633
00634
00635 }
00636
00637 VPUBLIC double Vacc_fastMolAcc(Vacc *thee, double center[VAPBS_DIM],
00638     double radius) {
00639     Vatom *atom;
00640     VaccSurf *surf;
00641     VclistCell *cell;
00642     int ipt, iatom, atomID;
00643     double dist2, rad2;
00644
00645     rad2 = radius*radius;
00646
00647 /* Check to see if the SAS has been defined */
00648 if (thee->surf == VNULL) Vacc_SASA(thee, radius);
00649
00650 /* Get the cell associated with this point */
00651 cell = Vclist_getCell(thee->clist, center);
00652 if (cell == VNULL) {
00653     Vnm_print(2, "Vacc_fastMolAcc: unexpected VNULL VclistCell!\n");
00654     return 1.0;
00655 }
00656
00657 /* Loop through all the atoms in the cell */
00658 for (iatom=0; iatom<cell->natoms; iatom++) {
00659     atom = cell->atoms[iatom];
00660     atomID = Vatom_getAtomID(atom);
00661     surf = thee->surf[atomID];
00662     /* Loop through all SAS points associated with this atom */
00663     for (ipt=0; ipt<surf->npts; ipt++) {
00664         /* See if we're within a probe radius of the point */
00665         dist2 = VSQR(center[0]-(surf->xpts[ipt]))
00666             + VSQR(center[1]-(surf->ypts[ipt]))
00667             + VSQR(center[2]-(surf->zpts[ipt]));
00668         if (dist2 < rad2) return 1.0;
00669     }
00670 }
00671
00672 /* If all else failed, we are not inside the molecular surface */
00673 return 0.0;
00674 }
00675
00676
00677
00678 #if defined(HAVE_MC_H)
00679 VPUBLIC void Vacc_writeGMV(Vacc *thee, double radius, int meth, Gem *gm,
00680     char *iodev, char *iofmt, char *iohost, char *iofile) {
00681     double *accVals[MAXV], coord[3];
00682     Vio *sock;
00683     int ivert, icoord;
00684
00685     for (ivert=0; ivert<MAXV; ivert++) accVals[ivert] = VNULL;
00686     accVals[0] = (void *)Vmem_malloc(thee->mem, Gem_numVV(gm), sizeof(double));
00687     accVals[1] = (void *)Vmem_malloc(thee->mem, Gem_numVV(gm), sizeof(double));
00688     for (ivert=0; ivert<Gem_numVV(gm); ivert++) {
00689         for (icoord=0; icoord<3; icoord++)
00690             coord[icoord] = VV_coord(Gem_VV(gm, ivert), icoord);
00691         if (meth == 0) {

```

```

00693         accVals[0][ivert] = Vacc_molAcc(thee, coord, radius);
00694         accVals[1][ivert] = Vacc_molAcc(thee, coord, radius);
00695     } else if (meth == 1) {
00696         accVals[0][ivert] = Vacc_ivdwAcc(thee, coord, radius);
00697         accVals[1][ivert] = Vacc_ivdwAcc(thee, coord, radius);
00698     } else if (meth == 2) {
00699         accVals[0][ivert] = Vacc_vdwAcc(thee, coord);
00700         accVals[1][ivert] = Vacc_vdwAcc(thee, coord);
00701     } else VASSERT(0);
00702 }
00703 sock = Vio_ctor(iodev, iofmt, iohost, iofile, "w");
00704 Gem_writeGMV(gm, sock, 1, accVals);
00705 Vio_dtor(&sock);
00706 Vmem_free(thee->mem, Gem_numVV(gm), sizeof(double),
00707           (void **)&(accVals[0]));
00708 Vmem_free(thee->mem, Gem_numVV(gm), sizeof(double),
00709           (void **)&(accVals[1]));
00710 }
00711 #endif /* defined(HAVE_MC_H) */
00712
00713 VPUBLIC double Vacc_SASA(Vacc *thee,
00714                        double radius
00715                        ) {
00716
00717     int i,
00718         natom;
00719     double area;
00720     /*apos; // gcc says unused
00721     Vatom *atom;
00722     VaccSurf *asurf;
00723
00724     time_t ts; // PCE: temp
00725     ts = clock();
00726
00727     //unsigned long long mbeg; // gcc says unused
00728
00729     natom = Valist_getNumberAtoms(thee->alist);
00730
00731     /* Check to see if we need to build the surface */
00732     if (thee->surf == VNULL) {
00733         thee->surf = Vmem_malloc(thee->mem, natom, sizeof(VaccSurf *));
00734
00735     #if defined(DEBUG_MAC_OSX_OCL) || defined(DEBUG_MAC_OSX_STANDARD)
00736     #include "mach_chud.h"
00737         machm_(&mbeg);
00738     #pragma omp parallel for private(i,atom)
00739     #endif
00740         for (i=0; i<natom; i++) {
00741             atom = Valist_getAtom(thee->alist, i);
00742             /* NOTE: RIGHT NOW WE DO THIS FOR THE ENTIRE MOLECULE WHICH IS
00743              * INCREDIBLY INEFFICIENT, PARTICULARLY DURING FOCUSING!!! */
00744             thee->surf[i] = Vacc_atomSurf(thee, atom, thee->refSphere,
00745                                         radius);
00746         }
00747     }
00748
00749     /* Calculate the area */
00750     area = 0.0;
00751     for (i=0; i<natom; i++) {
00752         atom = Valist_getAtom(thee->alist, i);
00753         asurf = thee->surf[i];
00754         /* See if this surface needs to be rebuilt */
00755         if (asurf->probe_radius != radius) {
00756             Vnm_print(2, "Vacc_SASA: Warning -- probe radius changed from %g to %g!\n",
00757                     asurf->probe_radius, radius);
00758             VaccSurf_dtor2(asurf);
00759             thee->surf[i] = Vacc_atomSurf(thee, atom, thee->refSphere, radius);
00760             asurf = thee->surf[i];
00761         }
00762         area += (asurf->area);
00763     }
00764
00765     #if defined(DEBUG_MAC_OSX_OCL) || defined(DEBUG_MAC_OSX_STANDARD)
00766     mets_(&mbeg, "Vacc_SASA - Parallel");
00767     #endif
00768
00769     Vnm_print(0, "Vacc_SASA: Time elapsed: %f\n", ((double)clock() - ts) / CLOCKS_PER_SEC);
00770     return area;
00771 }
00772 }
00773

```

```

00774 VPUBLIC double Vacc_totalSASA(Vacc *thee, double radius) {
00775
00776     return Vacc_SASA(thee, radius);
00777 }
00778
00779
00780 VPUBLIC double Vacc_atomSASA(Vacc *thee, double radius, Vatom *atom) {
00781
00782     VaccSurf *asurf;
00783     int id;
00784
00785     if (thee->surf == VNULL) Vacc_SASA(thee, radius);
00786
00787     id = Vatom_getAtomID(atom);
00788     asurf = thee->surf[id];
00789
00790     /* See if this surface needs to be rebuilt */
00791     if (asurf->probe_radius != radius) {
00792         Vnm_print(2, "Vacc_SASA: Warning -- probe radius changed from %g to %g!\n",
00793             asurf->probe_radius, radius);
00794         VaccSurf_dtor2(asurf);
00795         thee->surf[id] = Vacc_atomSurf(thee, atom, thee->refSphere, radius);
00796         asurf = thee->surf[id];
00797     }
00798
00799     return asurf->area;
00800 }
00801
00802
00803 VPUBLIC VaccSurf* VaccSurf_ctor(Vmem *mem, double probe_radius, int nsphere) {
00804     VaccSurf *thee;
00805
00806     //thee = Vmem_malloc(mem, 1, sizeof(Vacc) );
00807     thee = (VaccSurf*)calloc(1, sizeof(Vacc));
00808     VASSERT( VaccSurf_ctor2(thee, mem, probe_radius, nsphere) );
00809
00810     return thee;
00811 }
00812
00813 VPUBLIC int VaccSurf_ctor2(VaccSurf *thee, Vmem *mem, double probe_radius,
00814     int nsphere) {
00815
00816     if (thee == VNULL)
00817         return 0;
00818
00819     thee->mem = mem;
00820     thee->npts = nsphere;
00821     thee->probe_radius = probe_radius;
00822     thee->area = 0.0;
00823
00824     if (thee->npts > 0) {
00825         thee->xpts = Vmem_malloc(thee->mem, thee->npts, sizeof(double));
00826         thee->ypts = Vmem_malloc(thee->mem, thee->npts, sizeof(double));
00827         thee->zpts = Vmem_malloc(thee->mem, thee->npts, sizeof(double));
00828         thee->bpts = Vmem_malloc(thee->mem, thee->npts, sizeof(char));
00829     } else {
00830         thee->xpts = VNULL;
00831         thee->ypts = VNULL;
00832         thee->zpts = VNULL;
00833         thee->bpts = VNULL;
00834     }
00835
00836     return 1;
00837 }
00838
00839 VPUBLIC void VaccSurf_dtor(VaccSurf **thee) {
00840
00841     Vmem *mem;
00842
00843     if ((*thee) != VNULL) {
00844         mem = (*thee)->mem;
00845         VaccSurf_dtor2(*thee);
00846         //Vmem_free(mem, 1, sizeof(VaccSurf), (void **)thee);
00847         free(*thee);
00848         (*thee) = VNULL;
00849     }
00850 }
00851
00852
00853 VPUBLIC void VaccSurf_dtor2(VaccSurf *thee) {
00854

```

```

00855     if (thee->npts > 0) {
00856         Vmem_free(thee->mem, thee->npts, sizeof(double),
00857             (void **)&(thee->xpts));
00858         Vmem_free(thee->mem, thee->npts, sizeof(double),
00859             (void **)&(thee->ypts));
00860         Vmem_free(thee->mem, thee->npts, sizeof(double),
00861             (void **)&(thee->zpts));
00862         Vmem_free(thee->mem, thee->npts, sizeof(char),
00863             (void **)&(thee->bpts));
00864     }
00865 }
00866 }
00867
00868 VPUBLIC VaccSurf* Vacc_atomSurf(Vacc *thee, Vatom *atom,
00869     VaccSurf *ref, double prad) {
00870
00871     VaccSurf *surf;
00872     size_t i, j, npts;
00873     int atomID;
00874     double arad, rad, pos[3], *apos;
00875
00876     /* Get atom information */
00877     arad = Vatom_getRadius(atom);
00878     apos = Vatom_getPosition(atom);
00879     atomID = Vatom_getAtomID(atom);
00880
00881     if (arad < VSMALL) {
00882         return VaccSurf_ctor(thee->mem, prad, 0);
00883     }
00884
00885     rad = arad + prad;
00886
00887     /* Determine which points will contribute */
00888     npts = 0;
00889     for (i=0; i<ref->npts; i++) {
00890         /* Reset point flag: zero-radius atoms do not contribute */
00891         pos[0] = rad*(ref->xpts[i]) + apos[0];
00892         pos[1] = rad*(ref->ypts[i]) + apos[1];
00893         pos[2] = rad*(ref->zpts[i]) + apos[2];
00894         if (ivdwAccExclus(thee, pos, prad, atomID)) {
00895             npts++;
00896             ref->bpts[i] = (ref->bpts[i] < 1) + 1;
00897         } else {
00898             ref->bpts[i] <= 1;
00899         }
00900     }
00901
00902     /* Allocate space for the points */
00903     surf = VaccSurf_ctor(thee->mem, prad, npts);
00904
00905     /* Assign the points */
00906     j = 0;
00907     for (i=0; i<ref->npts; i++) {
00908         char flag = ref->bpts[i] & 1;
00909         ref->bpts[i] >= 1;
00910         if (flag) {
00911             surf->bpts[j] = 1;
00912             surf->xpts[j] = rad*(ref->xpts[i]) + apos[0];
00913             surf->ypts[j] = rad*(ref->ypts[i]) + apos[1];
00914             surf->zpts[j] = rad*(ref->zpts[i]) + apos[2];
00915             j++;
00916         }
00917     }
00918
00919     /* Assign the area */
00920     surf->area = 4.0*VPI*rad*rad*((double)(surf->npts))/((double)(ref->npts));
00921
00922     return surf;
00923 }
00924 }
00925
00926 VPUBLIC VaccSurf* VaccSurf_refSphere(Vmem *mem, int npts) {
00927
00928     VaccSurf *surf;
00929     int nactual, i, itheta, ntheta, iphi, nphimax, nphi;
00930     double frac;
00931     double sintheta, costheta, theta, dtheta;
00932     double sinphi, cosphi, phi, dphi;
00933
00934     /* Setup "constants" */
00935     frac = ((double)(npts))/4.0;

```

```

00936     ntheta = VRINT(VSQRT(Vunit_pi*frac));
00937     dtheta = Vunit_pi/((double)(ntheta));
00938     nphimax = 2*ntheta;
00939
00940     /* Count the actual number of points to be used */
00941     nactual = 0;
00942     for (itheta=0; itheta<ntheta; itheta++) {
00943         theta = dtheta*((double)(itheta));
00944         sintheta = VSIN(theta);
00945         costheta = VCOS(theta);
00946         nphi = VRINT(sintheta*nphimax);
00947         nactual += nphi;
00948     }
00949
00950     /* Allocate space for the points */
00951     surf = VaccSurf_ctor(mem, 1.0, nactual);
00952
00953     /* Clear out the boolean array */
00954     for (i=0; i<nactual; i++) surf->bpts[i] = 1;
00955
00956     /* Assign the points */
00957     nactual = 0;
00958     for (itheta=0; itheta<ntheta; itheta++) {
00959         theta = dtheta*((double)(itheta));
00960         sintheta = VSIN(theta);
00961         costheta = VCOS(theta);
00962         nphi = VRINT(sintheta*nphimax);
00963         if (nphi != 0) {
00964             dphi = 2*Vunit_pi/((double)(nphi));
00965             for (iphi=0; iphi<nphi; iphi++) {
00966                 phi = dphi*((double)(iphi));
00967                 sinphi = VSIN(phi);
00968                 cosphi = VCOS(phi);
00969                 surf->xpts[nactual] = cosphi * sintheta;
00970                 surf->ypts[nactual] = sinphi * sintheta;
00971                 surf->zpts[nactual] = costheta;
00972                 nactual++;
00973             }
00974         }
00975     }
00976
00977     surf->npts = nactual;
00978
00979     return surf;
00980 }
00981
00982 VPUBLIC VaccSurf* Vacc_atomSASPoints(Vacc *thee, double radius,
00983     Vatom *atom) {
00984
00985     VaccSurf *asurf = VNULL;
00986     int id;
00987
00988     if (thee->surf == VNULL) Vacc_SASA(thee, radius);
00989     id = Vatom_getAtomID(atom);
00990
00991     asurf = thee->surf[id];
00992
00993     /* See if this surface needs to be rebuilt */
00994     if (asurf->probe_radius != radius) {
00995         Vnm_print(2, "Vacc_SASA: Warning -- probe radius changed from %g to %g!\n",
00996             asurf->probe_radius, radius);
00997         VaccSurf_dtor2(asurf);
00998         thee->surf[id] = Vacc_atomSurf(thee, atom, thee->refSphere, radius);
00999         asurf = thee->surf[id];
01000     }
01001
01002     return asurf;
01003 }
01004 }
01005
01006 VPUBLIC void Vacc_splineAccGradAtomNorm4(Vacc *thee, double center[VAPBS_DIM],
01007     double win, double infrad, Vatom *atom, double *grad) {
01008
01009     int i;
01010     double dist, *apos, arad, sm, sm2, sm3, sm4, sm5, sm6, sm7;
01011     double e, e2, e3, e4, e5, e6, e7;
01012     double b, b2, b3, b4, b5, b6, b7;
01013     double c0, c1, c2, c3, c4, c5, c6, c7;
01014     double denom, mygrad;
01015     double mychi = 1.0; /* Char. func. value for given atom */
01016

```

```

01017     VASSERT(thee != NULL);
01018
01019     /* The grad is zero by default */
01020     for (i=0; i<VAPBS_DIM; i++) grad[i] = 0.0;
01021
01022     /* *** CALCULATE THE CHARACTERISTIC FUNCTION VALUE FOR THIS ATOM AND THE
01023        * *** MAGNITUDE OF THE FORCE *** */
01024     apos = Vatom_getPosition(atom);
01025     /* Zero-radius atoms don't contribute */
01026     if (Vatom_getRadius(atom) > 0.0) {
01027
01028         arad = Vatom_getRadius(atom);
01029         arad = arad + infrad;
01030         b = arad - win;
01031         e = arad + win;
01032
01033         e2 = e * e;
01034         e3 = e2 * e;
01035         e4 = e3 * e;
01036         e5 = e4 * e;
01037         e6 = e5 * e;
01038         e7 = e6 * e;
01039         b2 = b * b;
01040         b3 = b2 * b;
01041         b4 = b3 * b;
01042         b5 = b4 * b;
01043         b6 = b5 * b;
01044         b7 = b6 * b;
01045
01046         denom = e7 - 7.0*b*e6 + 21.0*b2*e5 - 35.0*e4*b3
01047             + 35.0*e3*b4 - 21.0*b5*e2 + 7.0*e*b6 - b7;
01048         c0 = b4*(35.0*e3 - 21.0*b*e2 + 7*e*b2 - b3)/denom;
01049         c1 = -140.0*b3*e3/denom;
01050         c2 = 210.0*e2*b2*(e + b)/denom;
01051         c3 = -140.0*e*b*(e2 + 3.0*b*e + b2)/denom;
01052         c4 = 35.0*(e3 + 9.0*b*e2 + + 9.0*e*b2 + b3)/denom;
01053         c5 = -84.0*(e2 + 3.0*b*e + b2)/denom;
01054         c6 = 70.0*(e + b)/denom;
01055         c7 = -20.0/denom;
01056
01057         dist = VSQRT(VSQR(apos[0]-center[0]) + VSQR(apos[1]-center[1])
01058             + VSQR(apos[2]-center[2]));
01059
01060         /* If we're inside an atom, the entire characteristic function
01061            * will be zero and the grad will be zero, so we can stop */
01062         if (dist < (arad - win)) return;
01063         /* Likewise, if we're outside the smoothing window, the characteristic
01064            * function is unity and the grad will be zero, so we can stop */
01065         else if (dist > (arad + win)) return;
01066         /* Account for floating point error at the border
01067            * NAB: COULDN'T THESE TESTS BE COMBINED AS BELOW
01068            * (Vacc_splineAccAtom)? */
01069         else if ((VABS(dist - (arad - win)) < VSMALL) ||
01070             (VABS(dist - (arad + win)) < VSMALL)) return;
01071         /* If we're inside the smoothing window */
01072         else {
01073             sm = dist;
01074             sm2 = sm * sm;
01075             sm3 = sm2 * sm;
01076             sm4 = sm3 * sm;
01077             sm5 = sm4 * sm;
01078             sm6 = sm5 * sm;
01079             sm7 = sm6 * sm;
01080             mychi = c0 + c1*sm + c2*sm2 + c3*sm3
01081                 + c4*sm4 + c5*sm5 + c6*sm6 + c7*sm7;
01082             mygrad = c1 + 2.0*c2*sm + 3.0*c3*sm2 + 4.0*c4*sm3
01083                 + 5.0*c5*sm4 + 6.0*c6*sm5 + 7.0*c7*sm6;
01084             if (mychi <= 0.0) {
01085                 /* Avoid numerical round off errors */
01086                 return;
01087             } else if (mychi > 1.0) {
01088                 /* Avoid numerical round off errors */
01089                 mychi = 1.0;
01090             }
01091         }
01092         /* Now assemble the grad vector */
01093         VASSERT(mychi > 0.0);
01094         for (i=0; i<VAPBS_DIM; i++)
01095             grad[i] = -(mygrad/mychi)*((center[i] - apos[i])/dist);
01096     }
01097 }

```

```

01098
01099 VPUBLIC void Vacc_splineAccGradAtomNorm3(Vacc *thee, double center[VAPBS_DIM],
01100                                           double win, double infrad, Vatom *atom, double *grad) {
01101
01102     int i;
01103     double dist, *apos, arad, sm, sm2, sm3, sm4, sm5;
01104     double e, e2, e3, e4, e5;
01105     double b, b2, b3, b4, b5;
01106     double c0, c1, c2, c3, c4, c5;
01107     double denom, mygrad;
01108     double mychi = 1.0;          /* Char. func. value for given atom */
01109
01110     VASSERT(thee != NULL);
01111
01112     /* The grad is zero by default */
01113     for (i=0; i<VAPBS_DIM; i++) grad[i] = 0.0;
01114
01115     /* *** CALCULATE THE CHARACTERISTIC FUNCTION VALUE FOR THIS ATOM AND THE
01116      * *** MAGNITUDE OF THE FORCE *** */
01117     apos = Vatom_getPosition(atom);
01118     /* Zero-radius atoms don't contribute */
01119     if (Vatom_getRadius(atom) > 0.0) {
01120
01121         arad = Vatom_getRadius(atom);
01122         arad = arad + infrad;
01123         b = arad - win;
01124         e = arad + win;
01125
01126         e2 = e * e;
01127         e3 = e2 * e;
01128         e4 = e3 * e;
01129         e5 = e4 * e;
01130         b2 = b * b;
01131         b3 = b2 * b;
01132         b4 = b3 * b;
01133         b5 = b4 * b;
01134
01135         denom = pow((e - b), 5.0);
01136         c0 = -10.0*e2*b3 + 5.0*e*b4 - b5;
01137         c1 = 30.0*e2*b2;
01138         c2 = -30.0*(e2*b + e*b2);
01139         c3 = 10.0*(e2 + 4.0*e*b + b2);
01140         c4 = -15.0*(e + b);
01141         c5 = 6;
01142         c0 = c0/denom;
01143         c1 = c1/denom;
01144         c2 = c2/denom;
01145         c3 = c3/denom;
01146         c4 = c4/denom;
01147         c5 = c5/denom;
01148
01149         dist = VSQRT(VSQR(apos[0]-center[0]) + VSQR(apos[1]-center[1])
01150                     + VSQR(apos[2]-center[2]));
01151
01152         /* If we're inside an atom, the entire characteristic function
01153          * will be zero and the grad will be zero, so we can stop */
01154         if (dist < (arad - win)) return;
01155         /* Likewise, if we're outside the smoothing window, the characteristic
01156          * function is unity and the grad will be zero, so we can stop */
01157         else if (dist > (arad + win)) return;
01158         /* Account for floating point error at the border
01159          * NAB: COULDN'T THESE TESTS BE COMBINED AS BELOW
01160          * (Vacc_splineAccAtom)? */
01161         else if ((VABS(dist - (arad - win)) < VSMALL) ||
01162                  (VABS(dist - (arad + win)) < VSMALL)) return;
01163         /* If we're inside the smoothing window */
01164         else {
01165             sm = dist;
01166             sm2 = sm * sm;
01167             sm3 = sm2 * sm;
01168             sm4 = sm3 * sm;
01169             sm5 = sm4 * sm;
01170             mychi = c0 + c1*sm + c2*sm2 + c3*sm3
01171                   + c4*sm4 + c5*sm5;
01172             mygrad = c1 + 2.0*c2*sm + 3.0*c3*sm2 + 4.0*c4*sm3
01173                   + 5.0*c5*sm4;
01174             if (mychi <= 0.0) {
01175                 /* Avoid numerical round off errors */
01176                 return;
01177             } else if (mychi > 1.0) {
01178                 /* Avoid numerical round off errors */

```

```

01179         mychi = 1.0;
01180     }
01181 }
01182 /* Now assemble the grad vector */
01183 VASSERT(mychi > 0.0);
01184 for (i=0; i<VAPBS_DIM; i++)
01185     grad[i] = -(mygrad/mychi)*((center[i] - apos[i])/dist);
01186 }
01187 }
01188
01189 /* ////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////// */
01190 // Routine:  Vacc_atomdSAV
01191 //
01192 // Purpose:  Calculates the vector valued atomic derivative of volume
01193 //
01194 // Args:     radius  The radius of the solvent probe in Angstroms
01195 //           iatom   Index of the atom in thee->alist
01196 //
01197 // Author:   Jason Wagoner
01198 //           Nathan Baker (original FORTRAN routine from UHBD by Brock Luty)
01200 VPUBLIC void Vacc_atomdSAV(Vacc *thee,
01201                          double srad,
01202                          Vatom *atom,
01203                          double *dSA
01204                          ) {
01205
01206     int ipt, iatom;
01207
01208     double area;
01209     double *tPos, tRad, vec[3];
01210     double dx,dy,dz;
01211     VaccSurf *ref;
01212     dx = 0.0;
01213     dy = 0.0;
01214     dz = 0.0;
01215     /* Get the atom information */
01216     ref = thee->refSphere;
01217     iatom = Vatom_getAtomID(atom);
01218
01219     dSA[0] = 0.0;
01220     dSA[1] = 0.0;
01221     dSA[2] = 0.0;
01222
01223     tPos = Vatom_getPosition(atom);
01224     tRad = Vatom_getRadius(atom);
01225
01226     if(tRad == 0.0) return;
01227
01228     area = 4.0*VPI*(tRad+srad)*(tRad+srad)/((double)(ref->npts));
01229     for (ipt=0; ipt<ref->npts; ipt++) {
01230         vec[0] = (tRad+srad)*ref->xpts[ipt] + tPos[0];
01231         vec[1] = (tRad+srad)*ref->ypts[ipt] + tPos[1];
01232         vec[2] = (tRad+srad)*ref->zpts[ipt] + tPos[2];
01233         if (ivdwAccExclus(thee, vec, srad, iatom)) {
01234             dx = dx+vec[0]-tPos[0];
01235             dy = dy+vec[1]-tPos[1];
01236             dz = dz+vec[2]-tPos[2];
01237         }
01238     }
01239
01240     if ((tRad+srad) != 0){
01241         dSA[0] = dx*area/(tRad+srad);
01242         dSA[1] = dy*area/(tRad+srad);
01243         dSA[2] = dz*area/(tRad+srad);
01244     }
01245
01246 }
01247
01248 /* Note: This is purely test code to make certain that the dSASA code is
01249     behaving properly. This function should NEVER be called by anyone
01250     other than an APBS developer at Wash U.
01251 */
01252 VPRIVATE double Vacc_SASAPos(Vacc *thee, double radius) {
01253
01254     int i, natom;
01255     double area;
01256     Vatom *atom;
01257     VaccSurf *asurf;
01258
01259     natom = Valist_getNumberAtoms(thee->alist);
01260

```



```

01261      /* Calculate the area */
01262      area = 0.0;
01263      for (i=0; i<natom; i++) {
01264          atom = Valist_getAtom(thee->alist, i);
01265          asurf = thee->surf[i];
01266
01267          VaccSurf_dtor2(asurf);
01268          thee->surf[i] = Vacc_atomSurf(thee, atom, thee->refSphere, radius);
01269          asurf = thee->surf[i];
01270          area += (asurf->area);
01271      }
01272
01273      return area;
01274  }
01275 }
01276
01277 VPRIVATE double Vacc_atomSASAPos(Vacc *thee,
01278                                  double radius,
01279                                  Vatom *atom, /* The atom being manipulated */
01280                                  int mode
01281                                  ) {
01282
01283     VaccSurf *asurf;
01284     int id;
01285     static int warned = 0;
01286
01287     if ((thee->surf == VNULL) || (mode == 1)){
01288         if(!warned){
01289             Vnm_print(2, "WARNING: Recalculating entire surface!!!!\n");
01290             warned = 1;
01291         }
01292         Vacc_SASAPos(thee, radius); // reinitialize before we can do anything about doing a calculation on
a repositioned atom
01293     }
01294
01295     id = Vatom_getAtomID(atom);
01296     asurf = thee->surf[id];
01297
01298     VaccSurf_dtor(&asurf);
01299     thee->surf[id] = Vacc_atomSurf(thee, atom, thee->refSphere, radius);
01300     asurf = thee->surf[id];
01301
01302     //printf("%s: Time elapsed: %f\n", __func__, ((double)clock() - ts) / CLOCKS_PER_SEC);
01303
01304     return asurf->area;
01305 }
01306
01307 /* ////////////////////////////////////////
01308 // Routine: Vacc_atomdSASA
01309 //
01310 // Purpose: Calculates the derivative of surface area with respect to atomic
01311 //           displacement using finite difference methods.
01312 //
01313 // Args:    radius The radius of the solvent probe in Angstroms
01314 //           iatom  Index of the atom in thee->alist
01315 //
01316 // Author:   Jason Wagoner
01317 //           David Gohara
01318 //           Nathan Baker (original FORTRAN routine from UHBD by Brock Luty)
01320 VPUBLIC void Vacc_atomdSASA(Vacc *thee,
01321                             double dpos,
01322                             double srاد,
01323                             Vatom *atom,
01324                             double *dSA
01325                             ) {
01326
01327     double *temp_Pos,
01328            tPos[3],
01329            axbl,
01330            axtl,
01331            aybl,
01332            aytl,
01333            azbl,
01334            aztl;
01335     VaccSurf *ref;
01336
01337     //printf("%s: entering\n", __func__);
01338     time_t ts;
01339     ts = clock();
01340
01341     /* Get the atom information */

```

```

01342     ref = thee->refSphere;
01343     temp_Pos = Vatom_getPosition(atom); // Get a pointer to the position object. You actually manipulate
the atom doing this...
01344
01345     tPos[0] = temp_Pos[0];
01346     tPos[1] = temp_Pos[1];
01347     tPos[2] = temp_Pos[2];
01348
01349     /* Shift by pos +/- on x */
01350     temp_Pos[0] -= dpos;
01351     axb1 = Vacc_atomSASAPos(thee, srاد, atom,0);
01352     temp_Pos[0] = tPos[0];
01353
01354     temp_Pos[0] += dpos;
01355     axtl = Vacc_atomSASAPos(thee, srاد, atom,0);
01356     temp_Pos[0] = tPos[0];
01357
01358     /* Shift by pos +/- on y */
01359     temp_Pos[1] -= dpos;
01360     ayb1 = Vacc_atomSASAPos(thee, srاد, atom,0);
01361     temp_Pos[1] = tPos[1];
01362
01363     temp_Pos[1] += dpos;
01364     ayt1 = Vacc_atomSASAPos(thee, srاد, atom,0);
01365     temp_Pos[1] = tPos[1];
01366
01367     /* Shift by pos +/- on z */
01368     temp_Pos[2] -= dpos;
01369     azb1 = Vacc_atomSASAPos(thee, srاد, atom,0);
01370     temp_Pos[2] = tPos[2];
01371
01372     temp_Pos[2] += dpos;
01373     aztl = Vacc_atomSASAPos(thee, srاد, atom,0);
01374     temp_Pos[2] = tPos[2];
01375
01376     /* Reset the atom SASA to zero displacement */
01377     Vacc_atomSASAPos(thee, srاد, atom,0);
01378
01379     /* Calculate the final value */
01380     dSA[0] = (axtl-axb1)/(2.0 * dpos);
01381     dSA[1] = (aytl-ayb1)/(2.0 * dpos);
01382     dSA[2] = (aztl-azb1)/(2.0 * dpos);
01383 }
01384
01385 /* Note: This is purely test code to make certain that the dSASA code is
01386     behaving properly. This function should NEVER be called by anyone
01387     other than an APBS developer at Wash U.
01388 */
01389 VPUBLIC void Vacc_totalAtomdSASA(Vacc *thee, double dpos, double srاد, Vatom *atom, double *dSA) {
01390
01391     int iatom;
01392     double *temp_Pos, tRad;
01393     double tPos[3];
01394     double axb1,axtl,ayb1,aytl,azb1,aztl;
01395     VaccSurf *ref;
01396
01397     /* Get the atom information */
01398     ref = thee->refSphere;
01399     temp_Pos = Vatom_getPosition(atom);
01400     tRad = Vatom_getRadius(atom);
01401     iatom = Vatom_getAtomID(atom);
01402
01403     dSA[0] = 0.0;
01404     dSA[1] = 0.0;
01405     dSA[2] = 0.0;
01406
01407     tPos[0] = temp_Pos[0];
01408     tPos[1] = temp_Pos[1];
01409     tPos[2] = temp_Pos[2];
01410
01411     /* Shift by pos +/- on x */
01412     temp_Pos[0] -= dpos;
01413     axb1 = Vacc_atomSASAPos(thee, srاد, atom, 1);
01414     temp_Pos[0] = tPos[0];
01415
01416     temp_Pos[0] += dpos;
01417     axtl = Vacc_atomSASAPos(thee, srاد, atom, 1);
01418     temp_Pos[0] = tPos[0];
01419
01420     /* Shift by pos +/- on y */
01421     temp_Pos[1] -= dpos;

```

```

01422     ayb1 = Vacc_atomSASAPos(thee, srاد, atom, 1);
01423     temp_Pos[1] = tPos[1];
01424
01425     temp_Pos[1] += dpos;
01426     ayt1 = Vacc_atomSASAPos(thee, srاد, atom, 1);
01427     temp_Pos[1] = tPos[1];
01428
01429     /* Shift by pos +/- on z */
01430     temp_Pos[2] -= dpos;
01431     azb1 = Vacc_atomSASAPos(thee, srاد, atom, 1);
01432     temp_Pos[2] = tPos[2];
01433
01434     temp_Pos[2] += dpos;
01435     azt1 = Vacc_atomSASAPos(thee, srاد, atom, 1);
01436     temp_Pos[2] = tPos[2];
01437
01438     /* Calculate the final value */
01439     dSA[0] = (axt1-axb1)/(2.0 * dpos);
01440     dSA[1] = (ayt1-ayb1)/(2.0 * dpos);
01441     dSA[2] = (azt1-azb1)/(2.0 * dpos);
01442 }
01443
01444 /* Note: This is purely test code to make certain that the dSASA code is
01445     behaving properly. This function should NEVER be called by anyone
01446     other than an APBS developer at Wash U.
01447 */
01448 VPUBLIC void Vacc_totalAtomdSAV(Vacc *thee, double dpos, double srاد, Vatom *atom, double *dSA, Vclist
    *clist) {
01449
01450     int iatom;
01451     double *temp_Pos, tRad;
01452     double tPos[3];
01453     double axb1,axt1,ayb1,ayt1,azb1,azt1;
01454     VaccSurf *ref;
01455
01456     /* Get the atom information */
01457     ref = thee->refSphere;
01458     temp_Pos = Vatom_getPosition(atom);
01459     tRad = Vatom_getRadius(atom);
01460     iatom = Vatom_getAtomID(atom);
01461
01462     dSA[0] = 0.0;
01463     dSA[1] = 0.0;
01464     dSA[2] = 0.0;
01465
01466     tPos[0] = temp_Pos[0];
01467     tPos[1] = temp_Pos[1];
01468     tPos[2] = temp_Pos[2];
01469
01470     /* Shift by pos +/- on x */
01471     temp_Pos[0] -= dpos;
01472     axb1 = Vacc_totalSAV(thee,clist, VNULL, srاد);
01473     temp_Pos[0] = tPos[0];
01474
01475     temp_Pos[0] += dpos;
01476     axt1 = Vacc_totalSAV(thee,clist, VNULL, srاد);
01477     temp_Pos[0] = tPos[0];
01478
01479     /* Shift by pos +/- on y */
01480     temp_Pos[1] -= dpos;
01481     ayb1 = Vacc_totalSAV(thee,clist, VNULL, srاد);
01482     temp_Pos[1] = tPos[1];
01483
01484     temp_Pos[1] += dpos;
01485     ayt1 = Vacc_totalSAV(thee,clist, VNULL, srاد);
01486     temp_Pos[1] = tPos[1];
01487
01488     /* Shift by pos +/- on z */
01489     temp_Pos[2] -= dpos;
01490     azb1 = Vacc_totalSAV(thee,clist, VNULL, srاد);
01491     temp_Pos[2] = tPos[2];
01492
01493     temp_Pos[2] += dpos;
01494     azt1 = Vacc_totalSAV(thee,clist, VNULL, srاد);
01495     temp_Pos[2] = tPos[2];
01496
01497     /* Calculate the final value */
01498     dSA[0] = (axt1-axb1)/(2.0 * dpos);
01499     dSA[1] = (ayt1-ayb1)/(2.0 * dpos);
01500     dSA[2] = (azt1-azb1)/(2.0 * dpos);
01501 }

```

```

01502
01503 VPUBLIC double Vacc_totalSAV(Vacc *thee, Vclist *clist, APOLparm *apolparm, double radius) {
01504
01505     int i;
01506     int npts[3];
01507
01508     double spacs[3], vec[3];
01509     double w, wx, wy, wz, len, fn, x, y, z, vol;
01510     double vol_density,sav;
01511     double *lower_corner, *upper_corner;
01512
01513     sav = 0.0;
01514     vol = 1.0;
01515     vol_density = 2.0;
01516
01517     lower_corner = clist->lower_corner;
01518     upper_corner = clist->upper_corner;
01519
01520     for (i=0; i<3; i++) {
01521         len = upper_corner[i] - lower_corner[i];
01522         vol *= len;
01523         fn = len*vol_density + 1;
01524         npts[i] = (int)ceil(fn);
01525         spacs[i] = len/((double)(npts[i])-1.0);
01526         if (apolparm != VNULL) {
01527             if (apolparm->setgrid) {
01528                 if (apolparm->grid[i] > spacs[i]) {
01529                     Vnm_print(2, "Vacc_totalSAV: Warning, your GRID value (%g) is larger than the
recommended value (%g)!\n",
                                apolparm->grid[i], spacs[i]);
01530                 }
01531                 spacs[i] = apolparm->grid[i];
01532             }
01533         }
01534     }
01535 }
01536
01537
01538 for (x=lower_corner[0]; x<=upper_corner[0]; x=x+spacs[0]) {
01539     if ( VABS(x - lower_corner[0]) < VSMALL) {
01540         wx = 0.5;
01541     } else if ( VABS(x - upper_corner[0]) < VSMALL) {
01542         wx = 0.5;
01543     } else {
01544         wx = 1.0;
01545     }
01546     vec[0] = x;
01547     for (y=lower_corner[1]; y<=upper_corner[1]; y=y+spacs[1]) {
01548         if ( VABS(y - lower_corner[1]) < VSMALL) {
01549             wy = 0.5;
01550         } else if ( VABS(y - upper_corner[1]) < VSMALL) {
01551             wy = 0.5;
01552         } else {
01553             wy = 1.0;
01554         }
01555         vec[1] = y;
01556         for (z=lower_corner[2]; z<=upper_corner[2]; z=z+spacs[2]) {
01557             if ( VABS(z - lower_corner[2]) < VSMALL) {
01558                 wz = 0.5;
01559             } else if ( VABS(z - upper_corner[2]) < VSMALL) {
01560                 wz = 0.5;
01561             } else {
01562                 wz = 1.0;
01563             }
01564             vec[2] = z;
01565
01566             w = wx*wy*wz;
01567
01568             sav += (w*(1.0-Vacc_ivdwAcc(thee, vec, radius)));
01569
01570             } /* z loop */
01571         } /* y loop */
01572     } /* x loop */
01573
01574     w = spacs[0]*spacs[1]*spacs[2];
01575     sav *= w;
01576
01577     return sav;
01578 }
01579
01580 int Vacc_wcaEnergyAtom(Vacc *thee, APOLparm *apolparm, Valist *alist,
01581                       Vclist *clist, int iatom, double *value) {

```

```

01582
01583     int i;
01584     int npts[3];
01585     int pad = 14;
01586
01587     int xmin, ymin, zmin;
01588     int xmax, ymax, zmax;
01589
01590     double sigma6, sigma12;
01591
01592     double spacs[3], vec[3];
01593     double w, wx, wy, wz, len, fn, x, y, z, vol;
01594     double x2,y2,z2,r;
01595     double vol_density, energy, rho, srad;
01596     double psig, epsilon, watepsilon, sigma, watsigma, eni, chi;
01597
01598     double *pos;
01599     double *lower_corner, *upper_corner;
01600
01601     Vatom *atom = VNULL;
01602     VASSERT(apolparm != VNULL);
01603
01604     energy = 0.0;
01605     vol = 1.0;
01606     vol_density = 2.0;
01607
01608     lower_corner = clist->lower_corner;
01609     upper_corner = clist->upper_corner;
01610
01611     atom = Valist_getAtom(alist, iatom);
01612     pos = Vatom_getPosition(atom);
01613
01614     /* Note: these are the original temporary water parameters... they have been
01615        replaced by entries in a parameter file:
01616     watsigma = 1.7683;
01617     watepsilon = 0.1521;
01618     watepsilon = watepsilon*4.184;
01619     */
01620
01621     srad = apolparm->srad;
01622     rho = apolparm->bconc;
01623     watsigma = apolparm->watsigma;
01624     watepsilon = apolparm->watepsilon;
01625     psig = atom->radius;
01626     epsilon = atom->epsilon;
01627     sigma = psig + watsigma;
01628     epsilon = VSQRT((epsilon * watepsilon));
01629
01630     /* parameters */
01631     sigma6 = VPOW(sigma,6);
01632     sigma12 = VPOW(sigma,12);
01633     /* OPLS-style radius: double sigmar = sigma*VPOW(2, (1.0/6.0)); */
01634
01635     xmin = pos[0] - pad;
01636     xmax = pos[0] + pad;
01637     ymin = pos[1] - pad;
01638     ymax = pos[1] + pad;
01639     zmin = pos[2] - pad;
01640     zmax = pos[2] + pad;
01641
01642     for (i=0; i<3; i++) {
01643         len = (upper_corner[i] + pad) - (lower_corner[i] - pad);
01644         vol *= len;
01645         fn = len*vol_density + 1;
01646         npts[i] = (int)ceil(fn);
01647         spacs[i] = 0.5;
01648         if (apolparm->setgrid) {
01649             if (apolparm->grid[i] > spacs[i]) {
01650                 Vnm_print(2, "Vacc_totalsAV: Warning, your GRID value (%g) is larger than the recommended
value (%g)!\n",
01651                     apolparm->grid[i], spacs[i]);
01652             }
01653             spacs[i] = apolparm->grid[i];
01654         }
01655     }
01656
01657     for (x=xmin; x<=xmax; x=x+spacs[0]) {
01658         if ( VABS(x - xmin) < VSMALL) {
01659             wx = 0.5;
01660         } else if ( VABS(x - xmax) < VSMALL) {
01661             wx = 0.5;

```

```

01662     } else {
01663         wx = 1.0;
01664     }
01665     vec[0] = x;
01666     for (y=ymin; y<=ymax; y=y+spacs[1]) {
01667         if ( VABS(y - ymin) < VSMALL) {
01668             wy = 0.5;
01669         } else if ( VABS(y - ymax) < VSMALL) {
01670             wy = 0.5;
01671         } else {
01672             wy = 1.0;
01673         }
01674         vec[1] = y;
01675         for (z=zmin; z<=zmax; z=z+spacs[2]) {
01676             if ( VABS(z - zmin) < VSMALL) {
01677                 wz = 0.5;
01678             } else if ( VABS(z - zmax) < VSMALL) {
01679                 wz = 0.5;
01680             } else {
01681                 wz = 1.0;
01682             }
01683             vec[2] = z;
01684
01685             w = wx*wy*wz;
01686
01687             chi = Vacc_ivdwAcc(thee, vec, srads);
01688
01689             if (VABS(chi) > VSMALL) {
01690
01691                 x2 = VSQR(vec[0]-pos[0]);
01692                 y2 = VSQR(vec[1]-pos[1]);
01693                 z2 = VSQR(vec[2]-pos[2]);
01694                 r = VSQRT(x2+y2+z2);
01695
01696                 if (r <= 14 && r >= sigma) {
01697                     eni = chi*rho*epsilon*(-2.0*sigma6/VPOW(r,6)+sigma12/VPOW(r,12));
01698                 } else if (r <= 14){
01699                     eni = -1.0*epsilon*chi*rho;
01700                 } else{
01701                     eni = 0.0;
01702                 }
01703             } else{
01704                 eni = 0.0;
01705             }
01706
01707             energy += eni*w;
01708
01709         } /* z loop */
01710     } /* y loop */
01711 } /* x loop */
01712
01713 w = spacs[0]*spacs[1]*spacs[2];
01714 energy *= w;
01715
01716 *value = energy;
01717
01718 return VRC_SUCCESS;
01719 }
01720
01721 VPUBLIC int Vacc_wcaEnergy(Vacc *acc, APOLparm *apolparm, Valist *alist,
01722                          Vclist *clist){
01723
01724     int iatom;
01725     int rc = 0;
01726
01727     double energy = 0.0;
01728     double tenergy = 0.0;
01729     double rho = apolparm->bconc;
01730
01731     /* Do a sanity check to make sure that watepsilon and watsigma are set
01732      * If not, return with an error. */
01733     if(apolparm->setwat == 0){
01734         Vnm_print(2,"Vacc_wcaEnergy: Error. No value was set for watsigma and watepsilon.\n");
01735         return VRC_FAILURE;
01736     }
01737
01738     if (VABS(rho) < VSMALL) {
01739         apolparm->wcaEnergy = tenergy;
01740         return 1;
01741     }
01742

```

```

01743     for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++){
01744         rc = Vacc_wcaEnergyAtom(acc, apolparm, alist, clist, iatom, &energy);
01745         if(rc == 0) return 0;
01746         tenergy += energy;
01747     }
01748
01749     apolparm->wcaEnergy = tenergy;
01750
01751     return VRC_SUCCESS;
01752 }
01753
01754
01755
01756 VPUBLIC int Vacc_wcaForceAtom(Vacc *thee,
01757                               APOLparm *apolparm,
01758                               Vclist *clist,
01759                               Vatom *atom,
01760                               double *force
01761                               ){
01762     int i,
01763         si,
01764         npts[3],
01765         pad = 14,
01766         xmin,
01767         ymin,
01768         zmin,
01769         xmax,
01770         ymax,
01771         zmax;
01772
01773     double sigma6,
01774            sigma12,
01775            spacs[3],
01776            vec[3],
01777            fpt[3],
01778            w,
01779            wx,
01780            wy,
01781            wz,
01782            len,
01783            fn,
01784            x,
01785            y,
01786            z,
01787            vol,
01788            x2,
01789            y2,
01790            z2,
01791            r,
01792            vol_density,
01793            fo,
01794            rho,
01795            srاد,
01796            psig,
01797            epsilon,
01798            watepsilon,
01799            sigma,
01800            watsigma,
01801            chi,
01802            *pos,
01803            *lower_corner,
01804            *upper_corner;
01805
01806     /* Allocate needed variables now that we've asserted required conditions. */
01807     time_t ts;
01808     ts = clock();
01809
01810     VASSERT(apolparm != VNULL);
01811
01812     /* Do a sanity check to make sure that watepsilon and watsigma are set
01813      * If not, return with an error. */
01814     if(apolparm->setwat == 0){
01815         Vnm_print(2,"Vacc_wcaEnergy: Error. No value was set for watsigma and watepsilon.\n");
01816         return VRC_FAILURE;
01817     }
01818
01819     vol = 1.0;
01820     vol_density = 2.0;
01821
01822     lower_corner = clist->lower_corner;
01823     upper_corner = clist->upper_corner;

```

```

01824
01825     pos = Vatom_getPosition(atom);
01826
01827     srad = apolparm->srad;
01828     rho = apolparm->bconc;
01829     watsigma = apolparm->watsigma;
01830     watepsilon = apolparm->watepsilon;
01831
01832     psig = atom->radius;
01833     epsilon = atom->epsilon;
01834     sigma = psig + watsigma;
01835     epsilon = VSQRT((epsilon * watepsilon));
01836
01837     /* parameters */
01838     sigma6 = VPOW(sigma,6);
01839     sigma12 = VPOW(sigma,12);
01840     /* OPLS-style radius: double sigmar = sigma*VPOW(2, (1.0/6.0)); */
01841
01842     for (i=0; i<3; i++) {
01843         len = (upper_corner[i] + pad) - (lower_corner[i] - pad);
01844         vol *= len;
01845         fn = len*vol_density + 1;
01846         npts[i] = (int)ceil(fn);
01847         spacs[i] = 0.5;
01848         force[i] = 0.0;
01849         if (apolparm->setgrid) {
01850             if (apolparm->grid[i] > spacs[i]) {
01851                 Vnm_print(2, "Vacc_totalsAV: Warning, your GRID value (%g) is larger than the recommended
value (%g)!\n",
01852                     apolparm->grid[i], spacs[i]);
01853             }
01854             spacs[i] = apolparm->grid[i];
01855         }
01856     }
01857
01858     xmin = pos[0] - pad;
01859     xmax = pos[0] + pad;
01860     ymin = pos[1] - pad;
01861     ymax = pos[1] + pad;
01862     zmin = pos[2] - pad;
01863     zmax = pos[2] + pad;
01864
01865     for (x=xmin; x<=xmax; x=x+spacs[0]) {
01866         if ( VABS(x - xmin) < VSMALL) {
01867             wx = 0.5;
01868         } else if ( VABS(x - xmax) < VSMALL) {
01869             wx = 0.5;
01870         } else {
01871             wx = 1.0;
01872         }
01873         vec[0] = x;
01874         for (y=ymin; y<=ymax; y=y+spacs[1]) {
01875             if ( VABS(y - ymin) < VSMALL) {
01876                 wy = 0.5;
01877             } else if ( VABS(y - ymax) < VSMALL) {
01878                 wy = 0.5;
01879             } else {
01880                 wy = 1.0;
01881             }
01882             vec[1] = y;
01883             for (z=zmin; z<=zmax; z=z+spacs[2]) {
01884                 if ( VABS(z - zmin) < VSMALL) {
01885                     wz = 0.5;
01886                 } else if ( VABS(z - zmax) < VSMALL) {
01887                     wz = 0.5;
01888                 } else {
01889                     wz = 1.0;
01890                 }
01891             }
01892             vec[2] = z;
01893
01894             w = wx*wy*wz;
01895
01896             chi = Vacc_ivdWAcc(thee, vec, srad);
01897
01898             if (chi != 0.0) {
01899                 x2 = VSQR(vec[0]-pos[0]);
01900                 y2 = VSQR(vec[1]-pos[1]);
01901                 z2 = VSQR(vec[2]-pos[2]);
01902                 r = VSQRT(x2+y2+z2);
01903

```



```

01904         if (r <= 14 && r >= sigma){
01905
01906             fo = 12.0*chi*rho*epsilon*(sigma6/VPOW(r,7)-sigma12/VPOW(r,13));
01907
01908             fpt[0] = -1.0*(pos[0]-vec[0])*fo/r;
01909             fpt[1] = -1.0*(pos[1]-vec[1])*fo/r;
01910             fpt[2] = -1.0*(pos[2]-vec[2])*fo/r;
01911
01912             }else {
01913                 for (si=0; si < 3; si++) fpt[si] = 0.0;
01914             }
01915         }else {
01916             for (si=0; si < 3; si++) fpt[si] = 0.0;
01917         }
01918
01919         for(i=0;i<3;i++){
01920             force[i] += (w*fpt[i]);
01921         }
01922     } /* z loop */
01923 } /* y loop */
01924 } /* x loop */
01925
01926 w = spacs[0]*spacs[1]*spacs[2];
01927 for(i=0;i<3;i++) force[i] *= w;
01928
01929 return VRC_SUCCESS;
01930
01931 }

```

9.52 src/generic/vacc.h File Reference

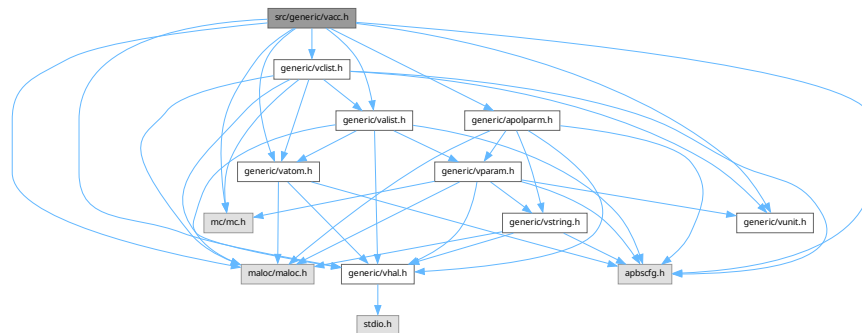
Contains declarations for class Vacc.

```

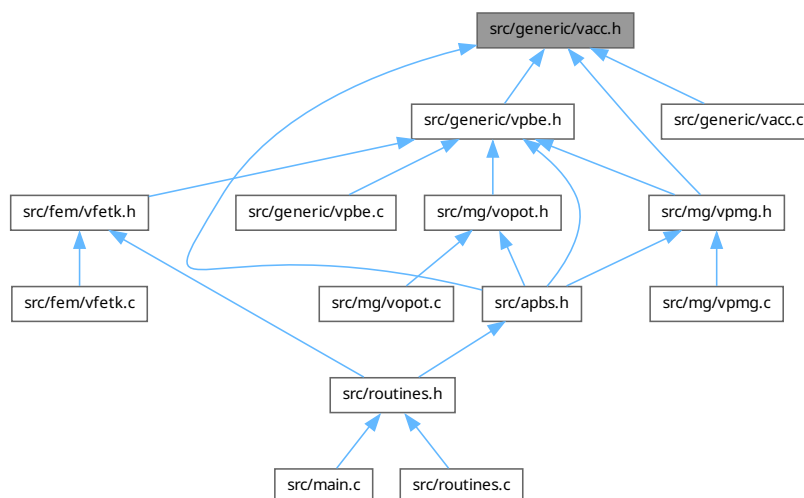
#include "apbscfg.h"
#include "malloc/malloc.h"
#include "mc/mc.h"
#include "generic/vhal.h"
#include "generic/valist.h"
#include "generic/vclist.h"
#include "generic/vatom.h"
#include "generic/vunit.h"
#include "generic/apolparm.h"

```

Include dependency graph for vacc.h:



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [sVaccSurf](#)
Surface object list of per-atom surface points.
- struct [sVacc](#)
Oracle for solvent- and ion-accessibility around a biomolecule.

Typedefs

- typedef struct [sVaccSurf](#) [VaccSurf](#)
Declaration of the VaccSurf class as the VaccSurf structure.
- typedef struct [sVacc](#) [Vacc](#)
Declaration of the Vacc class as the Vacc structure.

Functions

- VEXTERNC unsigned long int [Vacc_memChk](#) ([Vacc](#) *thee)
Get number of bytes in this object and its members.
- VEXTERNC [VaccSurf](#) * [VaccSurf_ctor](#) (Vmem *mem, double probe_radius, int nsphere)
Allocate and construct the surface object; do not assign surface points to positions.
- VEXTERNC int [VaccSurf_ctor2](#) ([VaccSurf](#) *thee, Vmem *mem, double probe_radius, int nsphere)
Construct the surface object using previously allocated memory; do not assign surface points to positions.
- VEXTERNC void [VaccSurf_dtor](#) ([VaccSurf](#) **thee)
Destroy the surface object and free its memory.
- VEXTERNC void [VaccSurf_dtor2](#) ([VaccSurf](#) *thee)
Destroy the surface object.
- VEXTERNC [VaccSurf](#) * [VaccSurf_refSphere](#) (Vmem *mem, int npts)
Set up an array of points for a reference sphere of unit radius.

- VEXTERNC `VaccSurf * Vacc_atomSurf (Vacc *thee, Vatom *atom, VaccSurf *ref, double probe_radius)`
Set up an array of points corresponding to the SAS due to a particular atom.
- VEXTERNC `Vacc * Vacc_ctor (Valist *alist, Vclist *clist, double surf_density)`
Construct the accessibility object.
- VEXTERNC `int Vacc_ctor2 (Vacc *thee, Valist *alist, Vclist *clist, double surf_density)`
FORTTRAN stub to construct the accessibility object.
- VEXTERNC `void Vacc_dtor (Vacc **thee)`
Destroy object.
- VEXTERNC `void Vacc_dtor2 (Vacc *thee)`
FORTTRAN stub to destroy object.
- VEXTERNC `double Vacc_vdwAcc (Vacc *thee, double center[VAPBS_DIM])`
Report van der Waals accessibility.
- VEXTERNC `double Vacc_ivdwAcc (Vacc *thee, double center[VAPBS_DIM], double radius)`
Report inflated van der Waals accessibility.
- VEXTERNC `double Vacc_molAcc (Vacc *thee, double center[VAPBS_DIM], double radius)`
Report molecular accessibility.
- VEXTERNC `double Vacc_fastMolAcc (Vacc *thee, double center[VAPBS_DIM], double radius)`
Report molecular accessibility quickly.
- VEXTERNC `double Vacc_splineAcc (Vacc *thee, double center[VAPBS_DIM], double win, double infrad)`
Report spline-based accessibility.
- VEXTERNC `void Vacc_splineAccGrad (Vacc *thee, double center[VAPBS_DIM], double win, double infrad, double *grad)`
Report gradient of spline-based accessibility.
- VEXTERNC `double Vacc_splineAccAtom (Vacc *thee, double center[VAPBS_DIM], double win, double infrad, Vatom *atom)`
Report spline-based accessibility for a given atom.
- VEXTERNC `void Vacc_splineAccGradAtomUnnorm (Vacc *thee, double center[VAPBS_DIM], double win, double infrad, Vatom *atom, double *force)`
Report gradient of spline-based accessibility with respect to a particular atom (see Vpmg_splineAccAtom)
- VEXTERNC `void Vacc_splineAccGradAtomNorm (Vacc *thee, double center[VAPBS_DIM], double win, double infrad, Vatom *atom, double *force)`
Report gradient of spline-based accessibility with respect to a particular atom normalized by the accessibility value due to that atom at that point (see Vpmg_splineAccAtom)
- VEXTERNC `void Vacc_splineAccGradAtomNorm4 (Vacc *thee, double center[VAPBS_DIM], double win, double infrad, Vatom *atom, double *force)`
Report gradient of spline-based accessibility with respect to a particular atom normalized by a 4th order accessibility value due to that atom at that point (see Vpmg_splineAccAtom)
- VEXTERNC `void Vacc_splineAccGradAtomNorm3 (Vacc *thee, double center[VAPBS_DIM], double win, double infrad, Vatom *atom, double *force)`
Report gradient of spline-based accessibility with respect to a particular atom normalized by a 3rd order accessibility value due to that atom at that point (see Vpmg_splineAccAtom)
- VEXTERNC `double Vacc_SASA (Vacc *thee, double radius)`
Build the solvent accessible surface (SAS) and calculate the solvent accessible surface area.
- VEXTERNC `double Vacc_totalSASA (Vacc *thee, double radius)`
Return the total solvent accessible surface area (SASA)
- VEXTERNC `double Vacc_atomSASA (Vacc *thee, double radius, Vatom *atom)`
Return the atomic solvent accessible surface area (SASA)
- VEXTERNC `VaccSurf * Vacc_atomSASPoints (Vacc *thee, double radius, Vatom *atom)`

Get the set of points for this atom's solvent-accessible surface.

- VEXTERNC void `Vacc_atomdSAV` (`Vacc *thee`, double radius, `Vatom *atom`, double *dSA)

Get the derivative of solvent accessible volume.

- VEXTERNC void `Vacc_atomdSASA` (`Vacc *thee`, double dpos, double radius, `Vatom *atom`, double *dSA)

Get the derivative of solvent accessible area.

- VEXTERNC void `Vacc_totalAtomdSASA` (`Vacc *thee`, double dpos, double radius, `Vatom *atom`, double *dSA)

Testing purposes only.

- VEXTERNC void `Vacc_totalAtomdSAV` (`Vacc *thee`, double dpos, double radius, `Vatom *atom`, double *dSA, `Vclist *clist`)

Total solvent accessible volume.

- VEXTERNC double `Vacc_totalSAV` (`Vacc *thee`, `Vclist *clist`, `APOLparm *apolparm`, double radius)

Return the total solvent accessible volume (SAV)

- VEXTERNC int `Vacc_wcaEnergy` (`Vacc *thee`, `APOLparm *apolparm`, `Valist *alist`, `Vclist *clist`)

Return the WCA integral energy.

- VEXTERNC int `Vacc_wcaForceAtom` (`Vacc *thee`, `APOLparm *apolparm`, `Vclist *clist`, `Vatom *atom`, double *force)

Return the WCA integral force.

- VEXTERNC int `Vacc_wcaEnergyAtom` (`Vacc *thee`, `APOLparm *apolparm`, `Valist *alist`, `Vclist *clist`, int iatom, double *value)

Calculate the WCA energy for an atom.

9.52.1 Detailed Description

Contains declarations for class `Vacc`.

Version

\$Id\$

Author

Nathan A. Baker

Attention

```
*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
* Nathan A. Baker (nathan.baker@pnnl.gov)
* Pacific Northwest National Laboratory
*
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*
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* THE POSSIBILITY OF SUCH DAMAGE.
*
*

```

Definition in file [vacc.h](#).

9.53 vacc.h

[Go to the documentation of this file.](#)

```

00001
00062 #ifndef _VACC_H_
00063 #define _VACC_H_
00064
00065 #include "apbscfg.h"
00066
00067 #include "malloc/malloc.h"
00068 #if defined(HAVE_MC_H)
00069 #include "mc/mc.h"
00070 #endif
00071
00072 #include "generic/vhal.h"
00073 #include "generic/valist.h"
00074 #include "generic/vclist.h"
00075 #include "generic/vatom.h"
00076 #include "generic/vunit.h"
00077 #include "generic/apolparm.h"
00078
00084 struct sVaccSurf {
00085     Vmem *mem;
00086     double *xpts;
00087     double *ypts;
00088     double *zpts;
00089     char *bpts;
00091     double area;
00092     int npts;
00093     double probe_radius;
00095 };
00096
00101 typedef struct sVaccSurf VaccSurf;
00102
00108 struct sVacc {
00109
00110     Vmem *mem;
00111     Valist *alist;
00112     Vclist *clist;
00113     int *atomFlags;
00116     VaccSurf *refSphere;
00117     VaccSurf **surf;
00120     Vset acc;
00122     double surf_density;
00125 };
00126
00131 typedef struct sVacc Vacc;

```

```
00132
00133 #if !defined(VINLINE_VACC)
00134
00140     VEXTERNC unsigned long int Vacc_memChk(
00141         Vacc *thee
00142     );
00143
00144 #else /* if defined(VINLINE_VACC) */
00145
00146 #    define Vacc_memChk(thee) (Vmem_bytes((thee)->mem))
00147
00148 #endif /* if !defined(VINLINE_VACC) */
00149
00157 VEXTERNC VaccSurf* VaccSurf_ctor(
00158     Vmem *mem,
00159     double probe_radius,
00160     int nsphere
00161 );
00162
00170 VEXTERNC int VaccSurf_ctor2(
00171     VaccSurf *thee,
00172     Vmem *mem,
00173     double probe_radius,
00174     int nsphere
00175 );
00176
00182 VEXTERNC void VaccSurf_dtor(
00183     VaccSurf **thee
00184 );
00185
00191 VEXTERNC void VaccSurf_dtor2(
00192     VaccSurf *thee
00193 );
00194
00209 VEXTERNC VaccSurf* VaccSurf_refSphere(
00210     Vmem *mem,
00211     int npts
00212 );
00213
00221 VEXTERNC VaccSurf* Vacc_atomSurf(
00222     Vacc *thee,
00223     Vatom *atom,
00224     VaccSurf *ref,
00226     double probe_radius
00227 );
00228
00233 VEXTERNC Vacc* Vacc_ctor(
00234     Valist *alist,
00235     Vclist *clist,
00237     double surf_density
00239 );
00240
00245 VEXTERNC int Vacc_ctor2(
00246     Vacc *thee,
00247     Valist *alist,
00248     Vclist *clist,
00250     double surf_density
00252 );
00253
00258 VEXTERNC void Vacc_dtor(
00259     Vacc **thee
00260 );
00261
00266 VEXTERNC void Vacc_dtor2(
00267     Vacc *thee
00268 );
00269
00280 VEXTERNC double Vacc_vdwAcc(
00281     Vacc *thee,
00282     double center[VAPBS_DIM]
00283 );
00284
00296 VEXTERNC double Vacc_ivdwAcc(
00297     Vacc *thee,
00298     double center[VAPBS_DIM],
00299     double radius
00300 );
00301
00316 VEXTERNC double Vacc_molAcc(
00317     Vacc *thee,
00318     double center[VAPBS_DIM],
```

```
00319         double radius
00320     );
00321
00340 VEXTERNC double Vacc_fastMolAcc(
00341     Vacc *thee,
00342     double center[VAPBS_DIM],
00343     double radius
00344 );
00345
00357 VEXTERNC double Vacc_splineAcc(
00358     Vacc *thee,
00359     double center[VAPBS_DIM],
00360     double win,
00361     double infrad
00362 );
00363
00369 VEXTERNC void Vacc_splineAccGrad(
00370     Vacc *thee,
00371     double center[VAPBS_DIM],
00372     double win,
00373     double infrad,
00374     double *grad
00375 );
00376
00388 VEXTERNC double Vacc_splineAccAtom(
00389     Vacc *thee,
00390     double center[VAPBS_DIM],
00391     double win,
00392     double infrad,
00393     Vatom *atom
00394 );
00395
00406 VEXTERNC void Vacc_splineAccGradAtomUnnorm(
00407     Vacc *thee,
00408     double center[VAPBS_DIM],
00409     double win,
00410     double infrad,
00411     Vatom *atom,
00412     double *force
00413 );
00414
00426 VEXTERNC void Vacc_splineAccGradAtomNorm(
00427     Vacc *thee,
00428     double center[VAPBS_DIM],
00429     double win,
00430     double infrad,
00431     Vatom *atom,
00432     double *force
00433 );
00434
00442 VEXTERNC void Vacc_splineAccGradAtomNorm4(
00443     Vacc *thee,
00444     double center[VAPBS_DIM],
00445     double win,
00446     double infrad,
00447     Vatom *atom,
00448     double *force
00449 );
00450
00458 VEXTERNC void Vacc_splineAccGradAtomNorm3(
00459     Vacc *thee,
00460     double center[VAPBS_DIM],
00461     double win,
00462     double infrad,
00463     Vatom *atom,
00464     double *force
00465 );
00466
00467
00477 VEXTERNC double Vacc_SASA(
00478     Vacc *thee,
00479     double radius
00480 );
00481
00489 VEXTERNC double Vacc_totalSASA(
00490     Vacc *thee,
00491     double radius
00492 );
00493
00501 VEXTERNC double Vacc_atomSASA(
00502     Vacc *thee,
```

```

00503         double radius,
00504         Vatom *atom
00505     );
00506
00513 VEXTERNC VaccSurf* Vacc_atomSASPoints(
00514     Vacc *thee,
00515     double radius,
00516     Vatom *atom
00517 );
00518
00524 VEXTERNC void Vacc_atomdSAV(
00525     Vacc *thee,
00526     double radius,
00527     Vatom *atom,
00528     double *dSA
00529 );
00530
00536 VEXTERNC void Vacc_atomdSASA(
00537     Vacc *thee,
00538     double dpos,
00539     double radius,
00540     Vatom *atom,
00541     double *dSA
00542 );
00543
00549 VEXTERNC void Vacc_totalAtomdSASA(
00550     Vacc *thee,
00551     double dpos,
00552     double radius,
00553     Vatom *atom,
00554     double *dSA
00555 );
00556
00562 VEXTERNC void Vacc_totalAtomdSAV(
00563     Vacc *thee,
00564     double dpos,
00565     double radius,
00566     Vatom *atom,
00567     double *dSA,
00568     Vclist *clist
00569 );
00570
00578 VEXTERNC double Vacc_totalSAV(
00579     Vacc *thee,
00580     Vclist *clist,
00581     APOLparm *apolparm,
00582     double radius
00583 );
00584
00585
00592 VEXTERNC int Vacc_wcaEnergy(
00593     Vacc *thee,
00594     APOLparm *apolparm,
00595     Valist *alist,
00596     Vclist *clist
00597 );
00604 VEXTERNC int Vacc_wcaForceAtom(Vacc *thee,
00605     APOLparm *apolparm,
00606     Vclist *clist,
00607     Vatom *atom,
00608     double *force
00609 );
00610
00616 VEXTERNC int Vacc_wcaEnergyAtom(
00617     Vacc *thee,
00618     APOLparm *apolparm,
00619     Valist *alist,
00620     Vclist *clist,
00621     int iatom,
00622     double *value
00623 );
00624
00625 #endif      /* ifndef _VACC_H_ */

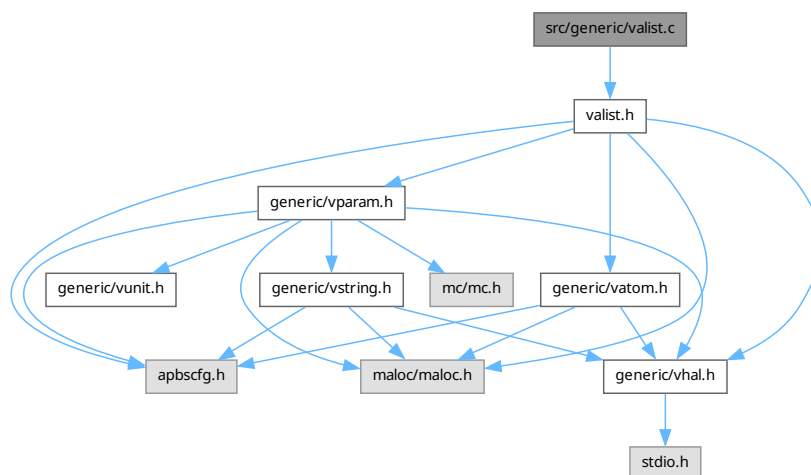
```

9.54 src/generic/valist.c File Reference

Class Valist methods.


```
#include "valist.h"
```

Include dependency graph for valist.c:



Functions

- VPUBLIC double [Valist_getCenterX](#) (Valist *thee)
Get x-coordinate of molecule center.
- VPUBLIC double [Valist_getCenterY](#) (Valist *thee)
Get y-coordinate of molecule center.
- VPUBLIC double [Valist_getCenterZ](#) (Valist *thee)
Get z-coordinate of molecule center.
- VPUBLIC Vatom * [Valist_getAtomList](#) (Valist *thee)
Get actual array of atom objects from the list.
- VPUBLIC int [Valist_getNumberAtoms](#) (Valist *thee)
Get number of atoms in the list.
- VPUBLIC Vatom * [Valist_getAtom](#) (Valist *thee, int i)
Get pointer to particular atom in list.
- VPUBLIC unsigned long int [Valist_memChk](#) (Valist *thee)
Get total memory allocated for this object and its members.
- VPUBLIC Valist * [Valist_ctor](#) ()
Construct the atom list object.
- VPUBLIC Vrc_Codes [Valist_ctor2](#) (Valist *thee)
FORTTRAN stub to construct the atom list object.
- VPUBLIC void [Valist_dtor](#) (Valist **thee)
Destroys atom list object.
- VPUBLIC void [Valist_dtor2](#) (Valist *thee)
FORTTRAN stub to destroy atom list object.
- VPRIVATE Vrc_Codes [Valist_readPDBSerial](#) (Valist *thee, Vio *sock, int *serial)
- VPRIVATE Vrc_Codes [Valist_readPDBAtomName](#) (Valist *thee, Vio *sock, char atomName[VMAX_ARGLEN])
- VPRIVATE Vrc_Codes [Valist_readPDBResidueName](#) (Valist *thee, Vio *sock, char resName[VMAX_ARGLEN])

- VPRIVATE Vrc_Codes [Valist_readPDBResidueNumber](#) ([Valist](#) *thee, [Vio](#) *sock, int *resSeq)
- VPRIVATE Vrc_Codes [Valist_readPDBAtomCoord](#) ([Valist](#) *thee, [Vio](#) *sock, double *coord)
- VPRIVATE Vrc_Codes [Valist_readPDBChargeRadius](#) ([Valist](#) *thee, [Vio](#) *sock, double *charge, double *radius)
- VPRIVATE Vrc_Codes [Valist_readPDB_throughXYZ](#) ([Valist](#) *thee, [Vio](#) *sock, int *serial, char atom←Name[VMAX_ARGLEN], char resName[VMAX_ARGLEN], int *resSeq, double *x, double *y, double *z)
- VPRIVATE [Vatom](#) * [Valist_getAtomStorage](#) ([Valist](#) *thee, [Vatom](#) **plist, int *pnlist, int *pnatoms)
- VPRIVATE Vrc_Codes [Valist_setAtomArray](#) ([Valist](#) *thee, [Vatom](#) **plist, int nlist, int natoms)
- VPUBLIC Vrc_Codes [Valist_readPDB](#) ([Valist](#) *thee, [Vparam](#) *param, [Vio](#) *sock)
Fill atom list with information from a PDB file.
- VPUBLIC Vrc_Codes [Valist_readPQR](#) ([Valist](#) *thee, [Vparam](#) *params, [Vio](#) *sock)
Fill atom list with information from a PQR file.
- VPUBLIC Vrc_Codes [Valist_readXML](#) ([Valist](#) *thee, [Vparam](#) *params, [Vio](#) *sock)
Fill atom list with information from an XML file.
- VPUBLIC Vrc_Codes [Valist_getStatistics](#) ([Valist](#) *thee)
Load up Valist with various statistics.

Variables

- VPRIVATE char * [Valist_whiteChars](#) = "\t\r\n"
- VPRIVATE char * [Valist_commChars](#) = "#%"
- VPRIVATE char * [Valist_xmlwhiteChars](#) = "\t\r\n<>"

9.54.1 Detailed Description

Class Valist methods.

Author

Nathan Baker

Version

\$Id\$

Attention

```
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*
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*
*
```

Definition in file [valist.c](#).

9.54.2 Function Documentation

9.54.2.1 Valist_getAtomStorage()

```
VPRIVATE Vatom * Valist_getAtomStorage (
    Valist * thee,
    Vatom ** plist,
    int * pntlist,
    int * pnatoms )
```

Definition at line [424](#) of file [valist.c](#).

9.54.2.2 Valist_readPDB_throughXYZ()

```
VPRIVATE Vrc_Codes Valist_readPDB_throughXYZ (
    Valist * thee,
    Vio * sock,
    int * serial,
    char atomName[VMAX_ARGLLEN],
    char resName[VMAX_ARGLLEN],
    int * resSeq,
    double * x,
    double * y,
    double * z )
```

Definition at line [344](#) of file [valist.c](#).

9.54.2.3 Valist_readPDBAtomCoord()

```
VPRIVATE Vrc_Codes Valist_readPDBAtomCoord (
    Valist * thee,
    Vio * sock,
    double * coord )
```

Definition at line [298](#) of file [valist.c](#).

9.54.2.4 Valist_readPDBAtomName()

```
VPRIVATE Vrc_Codes Valist_readPDBAtomName (
    Valist * thee,
    Vio * sock,
    char atomName[VMAX_ARGLLEN] )
```

Definition at line 206 of file [valist.c](#).

9.54.2.5 Valist_readPDBChargeRadius()

```
VPRIVATE Vrc_Codes Valist_readPDBChargeRadius (
    Valist * thee,
    Vio * sock,
    double * charge,
    double * radius )
```

Definition at line 316 of file [valist.c](#).

9.54.2.6 Valist_readPDBResidueName()

```
VPRIVATE Vrc_Codes Valist_readPDBResidueName (
    Valist * thee,
    Vio * sock,
    char resName[VMAX_ARGLLEN] )
```

Definition at line 224 of file [valist.c](#).

9.54.2.7 Valist_readPDBResidueNumber()

```
VPRIVATE Vrc_Codes Valist_readPDBResidueNumber (
    Valist * thee,
    Vio * sock,
    int * resSeq )
```

Definition at line 242 of file [valist.c](#).

9.54.2.8 Valist_readPDBSerial()

```
VPRIVATE Vrc_Codes Valist_readPDBSerial (
    Valist * thee,
    Vio * sock,
    int * serial )
```

Definition at line 186 of file [valist.c](#).

9.54.2.9 Valist_setAtomArray()

```
VPRIVATE Vrc_Codes Valist_setAtomArray (
    Valist * thee,
    Vatom ** plist,
    int nlist,
    int natoms )
```

Definition at line 480 of file [valist.c](#).

9.54.3 Variable Documentation

9.54.3.1 Valist_commChars

```
VPRIVATE char* Valist_commChars = "##"
```

Definition at line 61 of file [valist.c](#).

9.54.3.2 Valist_whiteChars

VPPRIVATE char* Valist_whiteChars = " \t\r\n"

Definition at line 60 of file [valist.c](#).

9.54.3.3 Valist_xmlwhiteChars

VPPRIVATE char* Valist_xmlwhiteChars = " \t\r\n<>"

Definition at line 62 of file [valist.c](#).

9.55 valist.c

[Go to the documentation of this file.](#)

```

00001
00056 #include "valist.h"
00057
00058 VEMBED(rcsid="$Id$")
00059
00060 VPPRIVATE char *Valist_whiteChars = " \t\r\n";
00061 VPPRIVATE char *Valist_commChars = "##";
00062 VPPRIVATE char *Valist_xmlwhiteChars = " \t\r\n<>";
00063
00064 #if !defined(VINLINE_VATOM)
00065
00066 VPUBLIC double Valist_getCenterX(Valist *thee) {
00067     if (thee == NULL) {
00068         Vnm_print(2, "Valist_getCenterX: Found null pointer when getting the center of X coordinate!\n");
00069         VASSERT(0);
00070     }
00071     return thee->center[0];
00072 }
00073
00074 }
00075
00076 VPUBLIC double Valist_getCenterY(Valist *thee) {
00077     if (thee == NULL) {
00078         Vnm_print(2, "Valist_getCenterY: Found null pointer when getting the center of Y coordinate!\n");
00079         VASSERT(0);
00080     }
00081     return thee->center[1];
00082 }
00083
00084 }
00085 VPUBLIC double Valist_getCenterZ(Valist *thee) {
00086     if (thee == NULL) {
00087         Vnm_print(2, "Valist_getCenterZ: Found null pointer when getting the center of Z coordinate!\n");
00088         VASSERT(0);
00089     }
00090     return thee->center[2];
00091 }
00092
00093 }
00094
00095 VPUBLIC Vatom* Valist_getAtomList(Valist *thee) {
00096     if (thee == NULL) {
00097         Vnm_print(2, "Valist_getAtomList: Found null pointer when getting the atom list!\n");
00098         VASSERT(0);
00099     }
00100     return thee->atoms;
00101 }
00102
00103 }
00104
00105 VPUBLIC int Valist_getNumberAtoms(Valist *thee) {
00106     if (thee == NULL) {
00107         Vnm_print(2, "Valist_getNumberAtoms: Found null pointer when getting the number of atoms!\n");
00108         VASSERT(0);
00109     }
00110     return thee->number;
00111 }
00112
00113 }
00114
00115 VPUBLIC Vatom* Valist_getAtom(Valist *thee, int i) {
00116

```

```

00117     if (thee == NULL) {
00118         Vnm_print(2, "Valist_getAtom: Found null pointer when getting atoms!\n");
00119         VASSERT(0);
00120     }
00121     if (i >= thee->number) {
00122         Vnm_print(2, "Valist_getAtom: Requested atom number (%d) outside of atom list range (%d)!\n", i,
thee->number);
00123         VASSERT(0);
00124     }
00125     return &(thee->atoms[i]);
00126 }
00127 }
00128
00129 VPUBLIC unsigned long int Valist_memChk(Valist *thee) {
00130
00131     if (thee == NULL) return 0;
00132     return Vmem_bytes(thee->vmem);
00133 }
00134 }
00135
00136 #endif /* if !defined(VINLINE_VATOM) */
00137
00138 VPUBLIC Valist* Valist_ctor() {
00139
00140     /* Set up the structure */
00141     Valist *thee = VNULL;
00142     thee = (Valist*)Vmem_malloc(VNULL, 1, sizeof(Valist));
00143     if (thee == VNULL) {
00144         Vnm_print(2, "Valist_ctor: Got NULL pointer when constructing the atom list object!\n");
00145         VASSERT(0);
00146     }
00147     if (Valist_ctor2(thee) != VRC_SUCCESS) {
00148         Vnm_print(2, "Valist_ctor: Error in constructing the atom list object!\n");
00149         VASSERT(0);
00150     }
00151
00152     return thee;
00153 }
00154
00155 VPUBLIC Vrc_Codes Valist_ctor2(Valist *thee) {
00156
00157     thee->atoms = VNULL;
00158     thee->number = 0;
00159
00160     /* Initialize the memory management object */
00161     thee->vmem = Vmem_ctor("APBS:VALIST");
00162
00163     return VRC_SUCCESS;
00164 }
00165 }
00166
00167 VPUBLIC void Valist_dtor(Valist **thee)
00168 {
00169     if ((*thee) != VNULL) {
00170         Valist_dtor2(*thee);
00171         Vmem_free(VNULL, 1, sizeof(Valist), (void **)thee);
00172         (*thee) = VNULL;
00173     }
00174 }
00175
00176 VPUBLIC void Valist_dtor2(Valist *thee) {
00177
00178     Vmem_free(thee->vmem, thee->number, sizeof(Vatom), (void **)&(thee->atoms));
00179     thee->atoms = VNULL;
00180     thee->number = 0;
00181
00182     Vmem_dtor(&(thee->vmem));
00183 }
00184
00185 /* Read serial number from PDB ATOM/HETATM field */
00186 VPRIVATE Vrc_Codes Valist_readPDBSerial(Valist *thee, Vio *sock, int *serial) {
00187
00188     char tok[VMAX_BUFSIZE];
00189     int ti = 0;
00190
00191     if (Vio_scanf(sock, "%s", tok) != 1) {
00192         Vnm_print(2, "Valist_readPDB: Ran out of tokens while parsing serial!\n");
00193         return VRC_FAILURE;
00194     }
00195     if (sscanf(tok, "%d", &ti) != 1) {
00196         Vnm_print(2, "Valist_readPDB: Unable to parse serial token (%s) as int!\n",

```

```
00197         tok);
00198     return VRC_FAILURE;
00199 }
00200 *serial = ti;
00201
00202     return VRC_SUCCESS;
00203 }
00204
00205 /* Read atom name from PDB ATOM/HETATM field */
00206 VPRIVATE Vrc_Codes Valist_readPDBAtomName(Valist *thee, Vio *sock,
00207     char atomName[VMAX_ARGLEN]) {
00208
00209     char tok[VMAX_BUFSIZE];
00210
00211     if (Vio_scanf(sock, "%s", tok) != 1) {
00212         Vnm_print(2, "Valist_readPDB: Ran out of tokens while parsing atom name!\n");
00213         return VRC_FAILURE;
00214     }
00215     if (strlen(tok) < VMAX_ARGLEN) strcpy(atomName, tok);
00216     else {
00217         Vnm_print(2, "Valist_readPDB: Atom name (%s) too long!\n", tok);
00218         return VRC_FAILURE;
00219     }
00220     return VRC_SUCCESS;
00221 }
00222
00223 /* Read residue name from PDB ATOM/HETATM field */
00224 VPRIVATE Vrc_Codes Valist_readPDBResidueName(Valist *thee, Vio *sock,
00225     char resName[VMAX_ARGLEN]) {
00226
00227     char tok[VMAX_BUFSIZE];
00228
00229     if (Vio_scanf(sock, "%s", tok) != 1) {
00230         Vnm_print(2, "Valist_readPDB: Ran out of tokens while parsing residue name!\n");
00231         return VRC_FAILURE;
00232     }
00233     if (strlen(tok) < VMAX_ARGLEN) strcpy(resName, tok);
00234     else {
00235         Vnm_print(2, "Valist_readPDB: Residue name (%s) too long!\n", tok);
00236         return VRC_FAILURE;
00237     }
00238     return VRC_SUCCESS;
00239 }
00240
00241 /* Read residue number from PDB ATOM/HETATM field */
00242 VPRIVATE Vrc_Codes Valist_readPDBResidueNumber(
00243     Valist *thee, Vio *sock, int *resSeq) {
00244
00245     char tok[VMAX_BUFSIZE];
00246     char *resstring;
00247     int ti = 0;
00248
00249     if (Vio_scanf(sock, "%s", tok) != 1) {
00250         Vnm_print(2, "Valist_readPDB: Ran out of tokens while parsing resSeq!\n");
00251         return VRC_FAILURE;
00252     }
00253     if (sscanf(tok, "%d", &ti) != 1) {
00254
00255         /* One of three things can happen here:
00256         1) There is a chainID in the line:   THR A   1
00257         2) The chainID is merged with resSeq: THR A1001
00258         3) An actual error:                 THR foo
00259
00260         */
00261
00262         if (strlen(tok) == 1) {
00263             /* Case 1: Chain ID Present
00264             Read the next field and hope its a float */
00265
00266             if (Vio_scanf(sock, "%s", tok) != 1) {
00267                 Vnm_print(2, "Valist_readPDB: Ran out of tokens while parsing resSeq!\n");
00268                 return VRC_FAILURE;
00269             }
00270             if (sscanf(tok, "%d", &ti) != 1) {
00271                 Vnm_print(2, "Valist_readPDB: Unable to parse resSeq token (%s) as int!\n",
00272                     tok);
00273                 return VRC_FAILURE;
00274             }
00275         } else {
00276             /* Case 2: Chain ID, merged string.
00277
```

```

00278             Move pointer forward past the chainID and check
00279             */
00280             //strcpy(resstring, tok);
00281             resstring = tok;
00282             resstring++;
00283
00284             if (sscanf(resstring, "%d", &ti) != 1) {
00285                 /* Case 3: More than one non-numeral char is present. Error.*/
00286                 Vnm_print(2, "Valist_readPDB: Unable to parse resSeq token (%s) as int!\n",
00287                     resstring);
00288                 return VRC_FAILURE;
00289             }
00290         }
00291     }
00292     *resSeq = ti;
00293
00294     return VRC_SUCCESS;
00295 }
00296
00297 /* Read atom coordinate from PDB ATOM/HETATM field */
00298 VPRIVATE Vrc_Codes Valist_readPDBAtomCoord(Valist *thee, Vio *sock, double *coord) {
00299     char tok[VMAX_BUFSIZE];
00300     double tf = 0;
00301
00302     if (Vio_sscanf(sock, "%s", tok) != 1) {
00303         Vnm_print(2, "Valist_readPDB: Ran out of tokens while parsing atom coordinate!\n");
00304         return VRC_FAILURE;
00305     }
00306     if (sscanf(tok, "%lf", &tf) != 1) {
00307         return VRC_FAILURE;
00308     }
00309     *coord = tf;
00310
00311     return VRC_SUCCESS;
00312 }
00313
00314 /* Read charge and radius from PQR ATOM/HETATM field */
00315 VPRIVATE Vrc_Codes Valist_readPDBChargeRadius(Valist *thee, Vio *sock,
00316     double *charge, double *radius) {
00317     char tok[VMAX_BUFSIZE];
00318     double tf = 0;
00319
00320     if (Vio_sscanf(sock, "%s", tok) != 1) {
00321         Vnm_print(2, "Valist_readPQR: Ran out of tokens while parsing charge!\n");
00322         return VRC_FAILURE;
00323     }
00324     if (sscanf(tok, "%lf", &tf) != 1) {
00325         return VRC_FAILURE;
00326     }
00327     *charge = tf;
00328
00329     if (Vio_sscanf(sock, "%s", tok) != 1) {
00330         Vnm_print(2, "Valist_readPQR: Ran out of tokens while parsing radius!\n");
00331         return VRC_FAILURE;
00332     }
00333     if (sscanf(tok, "%lf", &tf) != 1) {
00334         return VRC_FAILURE;
00335     }
00336     *radius = tf;
00337
00338     return VRC_SUCCESS;
00339 }
00340
00341 }
00342
00343 /* Read ATOM/HETATM field of PDB through the X/Y/Z fields */
00344 VPRIVATE Vrc_Codes Valist_readPDB_throughXYZ(
00345     Valist *thee,
00346     Vio *sock, /* Socket ready for reading */
00347     int *serial, /* Set to atom number */
00348     char atomName[VMAX_ARGLEN], /* Set to atom name */
00349     char resName[VMAX_ARGLEN], /* Set to residue name */
00350     int *resSeq, /* Set to residue number */
00351     double *x, /* Set to x-coordinate */
00352     double *y, /* Set to y-coordinate */
00353     double *z /* Set to z-coordinate */
00354 ) {
00355     int i, njunk, gotit;
00356
00357     int i, njunk, gotit;
00358

```



```
00359     /* Grab serial */
00360     if (Valist_readPDBSerial(thee, sock, serial) == VRC_FAILURE) {
00361         Vnm_print(2, "Valist_readPDB: Error while parsing serial!\n");
00362     }
00363
00364     /* Grab atom name */
00365     if (Valist_readPDBAtomName(thee, sock, atomName) == VRC_FAILURE) {
00366         Vnm_print(2, "Valist_readPDB: Error while parsing atom name!\n");
00367         return VRC_FAILURE;
00368     }
00369
00370     /* Grab residue name */
00371     if (Valist_readPDBResidueName(thee, sock, resName) == VRC_FAILURE) {
00372         Vnm_print(2, "Valist_readPDB: Error while parsing residue name!\n");
00373         return VRC_FAILURE;
00374     }
00375
00376     /* Grab residue number */
00377     if (Valist_readPDBResidueNumber(thee, sock, resSeq) == VRC_FAILURE) {
00378         Vnm_print(2, "Valist_readPDB: Error while parsing residue number!\n");
00379         return VRC_FAILURE;
00380     }
00381 }
00382
00383
00384 /* Read tokens until we find one that can be parsed as an atom
00385  * x-coordinate. We will allow njunk=1 intervening field that
00386  * cannot be parsed as a coordinate */
00387 njunk = 1;
00388 gotit = 0;
00389 for (i=0; i<(njunk+1); i++) {
00390     if (Valist_readPDBAtomCoord(thee, sock, x) == VRC_SUCCESS) {
00391         gotit = 1;
00392         break;
00393     }
00394 }
00395 if (!gotit) {
00396     Vnm_print(2, "Valist_readPDB: Can't find x!\n");
00397     return VRC_FAILURE;
00398 }
00399 /* Read y-coordinate */
00400 if (Valist_readPDBAtomCoord(thee, sock, y) == VRC_FAILURE) {
00401     Vnm_print(2, "Valist_readPDB: Can't find y!\n");
00402     return VRC_FAILURE;
00403 }
00404 /* Read z-coordinate */
00405 if (Valist_readPDBAtomCoord(thee, sock, z) == VRC_FAILURE) {
00406     Vnm_print(2, "Valist_readPDB: Can't find z!\n");
00407     return VRC_FAILURE;
00408 }
00409
00410 #if 0 /* Set to 1 if you want to debug */
00411     Vnm_print(1, "Valist_readPDB: serial = %d\n", *serial);
00412     Vnm_print(1, "Valist_readPDB: atomName = %s\n", atomName);
00413     Vnm_print(1, "Valist_readPDB: resName = %s\n", resName);
00414     Vnm_print(1, "Valist_readPDB: resSeq = %d\n", *resSeq);
00415     Vnm_print(1, "Valist_readPDB: pos = (%g, %g, %g)\n",
00416             *x, *y, *z);
00417 #endif
00418
00419     return VRC_SUCCESS;
00420 }
00421
00422 /* Get a the next available atom storage location, increasing the storage
00423  * space if necessary. Return VNULL if something goes wrong. */
00424 VPRIVATE Vatom* Valist_getAtomStorage(
00425     Valist *thee,
00426     Vatom **plist, /* Pointer to existing list of atoms */
00427     int *pnlist, /* Size of existing list, may be changed */
00428     int *pnatoms /* Existing number of atoms in list; incremented
00429                  before exit */
00430 ) {
00431
00432     Vatom *oldList, *newList, *theList;
00433     Vatom *oldAtom, *newAtom;
00434     int iatom, inext, oldLength, newLength, natoms;
00435
00436     newList = VNULL;
00437
00438     /* See if we need more space */
00439     if (*pnatoms >= *pnlist) {
```

```

00440
00441     /* Double the storage space */
00442     oldLength = *pnlist;
00443     newLength = 2*oldLength;
00444     newList = (Vatom*)Vmem_malloc(thee->vmem, newLength, sizeof(Vatom));
00445     oldList = *plist;
00446
00447     /* Check the allocation */
00448     if (newList == VNULL) {
00449         Vnm_print(2, "Valist_readPDB: failed to allocate space for %d (Vatom)s!\n", newLength);
00450         return VNULL;
00451     }
00452
00453     /* Copy the atoms over */
00454     natoms = *pnatoms;
00455     for (iatom=0; iatom<natoms; iatom++) {
00456         oldAtom = &(oldList[iatom]);
00457         newAtom = &(newList[iatom]);
00458         Vatom_copyTo(oldAtom, newAtom);
00459         Vatom_dtor2(oldAtom);
00460     }
00461
00462     /* Free the old list */
00463     Vmem_free(thee->vmem, oldLength, sizeof(Vatom), (void **)plist);
00464
00465     /* Copy new list to plist */
00466     *plist = newList;
00467     *pnlist = newLength;
00468 }
00469
00470 theList = *plist;
00471 inext = *pnatoms;
00472
00473 /* Get the next available spot and increment counters */
00474 newAtom = &(theList[inext]);
00475 *pnatoms = inext + 1;
00476
00477 return newAtom;
00478 }
00479
00480 VPRIVATE Vrc_Codes Valist_setAtomArray(Valist *thee,
00481     Vatom **plist, /* Pointer to list of atoms to store */
00482     int nlist, /* Length of list */
00483     int natoms /* Number of real atom entries in list */
00484 ) {
00485
00486     Vatom *list, *newAtom, *oldAtom;
00487     int i;
00488
00489     list = *plist;
00490
00491     /* Allocate necessary space */
00492     thee->number = 0;
00493     thee->atoms = (Vatom*)Vmem_malloc(thee->vmem, natoms, sizeof(Vatom));
00494     if (thee->atoms == VNULL) {
00495         Vnm_print(2, "Valist_readPDB: Unable to allocate space for %d (Vatom)s!\n",
00496             natoms);
00497         return VRC_FAILURE;
00498     }
00499     thee->number = natoms;
00500
00501     /* Copy over data */
00502     for (i=0; i<thee->number; i++) {
00503         newAtom = &(thee->atoms[i]);
00504         oldAtom = &(list[i]);
00505         Vatom_copyTo(oldAtom, newAtom);
00506         Vatom_dtor2(oldAtom);
00507     }
00508
00509     /* Free old array */
00510     Vmem_free(thee->vmem, nlist, sizeof(Vatom), (void **)plist);
00511
00512     return VRC_SUCCESS;
00513 }
00514
00515 VPUBLIC Vrc_Codes Valist_readPDB(Valist *thee, Vparam *param, Vio *sock) {
00516
00517     /* WE DO NOT DIRECTLY CONFORM TO PDB STANDARDS -- TO ALLOW LARGER FILES, WE
00518      * REQUIRE ALL FIELDS TO BE WHITESPACE DELIMITED */
00519
00520     Vatom *atoms = VNULL;

```

```
00521     Vatom *nextAtom = VNULL;
00522     Vparam_AtomData *atomData = VNULL;
00523
00524     char tok[VMAX_BUFSIZE];
00525     char atomName[VMAX_ARGLEN], resName[VMAX_ARGLEN];
00526
00527     int nlist, natoms, serial, resSeq;
00528
00529     double x, y, z, charge, radius, epsilon;
00530     double pos[3];
00531
00532     if (thee == VNULL) {
00533         Vnm_print(2, "Valist_readPDB: Got NULL pointer when reading PDB file!\n");
00534         VASSERT(0);
00535     }
00536     thee->number = 0;
00537
00538     Vio_setWhiteChars(sock, Valist_whiteChars);
00539     Vio_setCommChars(sock, Valist_commChars);
00540
00541     /* Allocate some initial space for the atoms */
00542     nlist = 200;
00543     atoms = (Vatom*)Vmem_malloc(thee->vmem, nlist, sizeof(Vatom));
00544
00545     natoms = 0;
00546     /* Read until we run out of lines */
00547     while (Vio_scanf(sock, "%s", tok) == 1) {
00548
00549         /* Parse only ATOM/HETATOM fields */
00550         if ((Vstring_strcasecmp(tok, "ATOM") == 0) ||
00551             (Vstring_strcasecmp(tok, "HETATM") == 0)) {
00552
00553             /* Read ATOM/HETATM field of PDB through the X/Y/Z fields */
00554             if (Valist_readPDB_throughXYZ(thee, sock, &serial, atomName,
00555                 resName, &resSeq, &x, &y, &z) == VRC_FAILURE) {
00556                 Vnm_print(2, "Valist_readPDB: Error parsing atom %d!\n",
00557                     serial);
00558                 return VRC_FAILURE;
00559             }
00560
00561             /* Try to find the parameters. */
00562             atomData = Vparam_getAtomData(param, resName, atomName);
00563             if (atomData == VNULL) {
00564                 Vnm_print(2, "Valist_readPDB: Couldn't find parameters for \
00565 atom = %s, residue = %s\n", atomName, resName);
00566                 return VRC_FAILURE;
00567             }
00568             charge = atomData->charge;
00569             radius = atomData->radius;
00570             epsilon = atomData->epsilon;
00571
00572             /* Get pointer to next available atom position */
00573             nextAtom = Valist_getAtomStorage(thee, &atoms, &nlist, &natoms);
00574             if (nextAtom == VNULL) {
00575                 Vnm_print(2, "Valist_readPDB: Error in allocating spacing for atoms!\n");
00576                 return VRC_FAILURE;
00577             }
00578
00579             /* Store the information */
00580             pos[0] = x; pos[1] = y; pos[2] = z;
00581             Vatom_setPosition(nextAtom, pos);
00582             Vatom_setCharge(nextAtom, charge);
00583             Vatom_setRadius(nextAtom, radius);
00584             Vatom_setEpsilon(nextAtom, epsilon);
00585             Vatom_setAtomID(nextAtom, natoms-1);
00586             Vatom_setResName(nextAtom, resName);
00587             Vatom_setAtomName(nextAtom, atomName);
00588
00589             } /* if ATOM or HETATM */
00590     } /* while we haven't run out of tokens */
00591
00592     Vnm_print(0, "Valist_readPDB: Counted %d atoms\n", natoms);
00593     fflush(stdout);
00594
00595     /* Store atoms internally */
00596     if (Valist_setAtomArray(thee, &atoms, nlist, natoms) == VRC_FAILURE) {
00597         Vnm_print(2, "Valist_readPDB: unable to store atoms!\n");
00598         return VRC_FAILURE;
00599     }
00600
00601     return Valist_getStatistics(thee);
```

```

00602
00603
00604 }
00605
00606 VPUBLIC Vrc_Codes Valist_readPQR(Valist *thee, Vparam *params, Vio *sock) {
00607
00608     /* WE DO NOT DIRECTLY CONFORM TO PDB STANDARDS -- TO ALLOW LARGER FILES, WE
00609      * REQUIRE ALL FIELDS TO BE WHITESPACE DELIMITED */
00610
00611
00612     Vatom *atoms = VNULL;
00613     Vatom *nextAtom = VNULL;
00614     Vparam_AtomData *atomData = VNULL;
00615
00616     char tok[VMAX_BUFSIZE];
00617     char atomName[VMAX_ARGLEN], resName[VMAX_ARGLEN];
00618     char chs[VMAX_BUFSIZE];
00619
00620     int use_params = 0;
00621     int nlist, natoms, serial, resSeq;
00622
00623     double x, y, z, charge, radius, epsilon;
00624     double pos[3];
00625
00626     epsilon = 0.0;
00627
00628     if (thee == VNULL) {
00629         Vnm_print(2, "Valist_readPQR: Got NULL pointer when reading PQR file!\n");
00630         VASSERT(0);
00631     }
00632     thee->number = 0;
00633
00634     Vio_setWhiteChars(sock, Valist_whiteChars);
00635     Vio_setCommChars(sock, Valist_commChars);
00636
00637     /* Allocate some initial space for the atoms */
00638     nlist = 200;
00639     atoms = (Vatom*)Vmem_malloc(thee->vmem, nlist, sizeof(Vatom));
00640
00641     /* Check if we are using a parameter file or not */
00642     if(params != VNULL) use_params = 1;
00643
00644     natoms = 0;
00645     /* Read until we run out of lines */
00646     while (Vio_scanf(sock, "%s", tok) == 1) {
00647
00648         /* Parse only ATOM/HETATOM fields */
00649         if ((Vstring_strcasecmp(tok, "ATOM") == 0) ||
00650             (Vstring_strcasecmp(tok, "HETATM") == 0)) {
00651
00652             /* Read ATOM/HETATM field of PDB through the X/Y/Z fields */
00653             if (Valist_readPDB_throughXYZ(thee, sock, &serial, atomName,
00654                 resName, &resSeq, &x, &y, &z) == VRC_FAILURE) {
00655                 Vnm_print(2, "Valist_readPQR: Error parsing atom %d!\n", serial);
00656                 Vnm_print(2, "Please double check this atom in the pqr file, e.g., make sure there are no
concatenated fields.\n");
00657                 return VRC_FAILURE;
00658             }
00659
00660             /* Read Q/R fields */
00661             if (Valist_readPDBChargeRadius(thee, sock, &charge, &radius) == VRC_FAILURE) {
00662                 Vnm_print(2, "Valist_readPQR: Error parsing atom %d!\n",
00663                     serial);
00664                 Vnm_print(2, "Please double check this atom in the pqr file, e.g., make sure there are no
concatenated fields.\n");
00665                 return VRC_FAILURE;
00666             }
00667
00668             if(use_params){
00669                 /* Try to find the parameters. */
00670                 atomData = Vparam_getAtomData(params, resName, atomName);
00671                 if (atomData == VNULL) {
00672                     Vnm_print(2, "Valist_readPDB: Couldn't find parameters for \
00673 atom = %s, residue = %s\n", atomName, resName);
00674                     return VRC_FAILURE;
00675                 }
00676                 charge = atomData->charge;
00677                 radius = atomData->radius;
00678                 epsilon = atomData->epsilon;
00679             }
00680

```

```

00681         /* Get pointer to next available atom position */
00682         nextAtom = Valist_getAtomStorage(thee, &atoms, &nlist, &natoms);
00683         if (nextAtom == VNULL) {
00684             Vnm_print(2, "Valist_readPQR: Error in allocating spacing for atoms!\n");
00685             return VRC_FAILURE;
00686         }
00687
00688         /* Store the information */
00689         pos[0] = x; pos[1] = y; pos[2] = z;
00690         Vatom_setPosition(nextAtom, pos);
00691         Vatom_setCharge(nextAtom, charge);
00692         Vatom_setRadius(nextAtom, radius);
00693         Vatom_setEpsilon(nextAtom, epsilon);
00694         Vatom_setAtomID(nextAtom, natoms-1);
00695         Vatom_setResName(nextAtom, resName);
00696         Vatom_setAtomName(nextAtom, atomName);
00697
00698     } /* if ATOM or HETATM */
00699     else {
00700         /*
00701          * nop
00702          * Note that if we find a line that starts with something that's not
00703          * ATOM or HETATM we'll just keep parsing strings until we find one
00704          * of the acceptable keywords.
00705          * Extraordinary measures are not necessary, and only add to the
00706          * befuddlement.
00707          */
00708     }
00709 } /* while we haven't run out of tokens */
00710
00711 Vnm_print(0, "Valist_readPQR: Counted %d atoms\n", natoms);
00712 fflush(stdout);
00713
00714 /* Store atoms internally */
00715 if (Valist_setAtomArray(thee, &atoms, nlist, natoms) == VRC_FAILURE) {
00716     Vnm_print(2, "Valist_readPDB: unable to store atoms!\n");
00717     return VRC_FAILURE;
00718 }
00719
00720 return Valist_getStatistics(thee);
00721
00722 }
00723
00724
00725 VPUBLIC Vrc_Codes Valist_readXML(Valist *thee, Vparam *params, Vio *sock) {
00726
00727     Vatom *atoms = VNULL;
00728     Vatom *nextAtom = VNULL;
00729
00730     char tok[VMAX_BUFSIZE];
00731     char endtag[VMAX_BUFSIZE];
00732
00733     int nlist, natoms;
00734     int xset, yset, zset, chgset, radset;
00735
00736     double x, y, z, charge, radius, dtmp;
00737     double pos[3];
00738
00739     if (thee == VNULL) {
00740         Vnm_print(2, "Valist_readXML: Got NULL pointer when reading XML file!\n");
00741         VASSERT(0);
00742     }
00743     thee->number = 0;
00744
00745     Vio_setWhiteChars(sock, Valist_xmlwhiteChars);
00746     Vio_setCommChars(sock, Valist_commChars);
00747
00748     /* Allocate some initial space for the atoms */
00749     nlist = 200;
00750     atoms = (Vatom*)Vmem_malloc(thee->vmem, nlist, sizeof(Vatom));
00751
00752     /* Initialize some variables */
00753     natoms = 0;
00754     xset = 0;
00755     yset = 0;
00756     zset = 0;
00757     chgset = 0;
00758     radset = 0;
00759     strcpy(endtag, "/");
00760
00761     if (params == VNULL) {

```

```

00762         Vnm_print(1, "\nValist_readXML: Warning Warning Warning Warning Warning\n");
00763         Vnm_print(1, "Valist_readXML: The use of XML input files with parameter\n");
00764         Vnm_print(1, "Valist_readXML: files is currently not supported.\n");
00765         Vnm_print(1, "Valist_readXML: Warning Warning Warning Warning Warning\n\n");
00766     }
00767
00768     /* Read until we run out of lines */
00769     while (Vio_scanf(sock, "%s", tok) == 1) {
00770
00771         /* The first tag taken is the start tag - save it to detect end */
00772         if (Vstring_strcasecmp(endtag, "/") == 0) strcat(endtag, tok);
00773
00774         if (Vstring_strcasecmp(tok, "x") == 0) {
00775             Vio_scanf(sock, "%s", tok);
00776             if (sscanf(tok, "%lf", &dtmp) != 1) {
00777                 Vnm_print(2, "Valist_readXML: Unexpected token (%s) while \
00778 reading x!\n", tok);
00779                 return VRC_FAILURE;
00780             }
00781             x = dtmp;
00782             xset = 1;
00783         } else if (Vstring_strcasecmp(tok, "y") == 0) {
00784             Vio_scanf(sock, "%s", tok);
00785             if (sscanf(tok, "%lf", &dtmp) != 1) {
00786                 Vnm_print(2, "Valist_readXML: Unexpected token (%s) while \
00787 reading y!\n", tok);
00788                 return VRC_FAILURE;
00789             }
00790             y = dtmp;
00791             yset = 1;
00792         } else if (Vstring_strcasecmp(tok, "z") == 0) {
00793             Vio_scanf(sock, "%s", tok);
00794             if (sscanf(tok, "%lf", &dtmp) != 1) {
00795                 Vnm_print(2, "Valist_readXML: Unexpected token (%s) while \
00796 reading z!\n", tok);
00797                 return VRC_FAILURE;
00798             }
00799             z = dtmp;
00800             zset = 1;
00801         } else if (Vstring_strcasecmp(tok, "charge") == 0) {
00802             Vio_scanf(sock, "%s", tok);
00803             if (sscanf(tok, "%lf", &dtmp) != 1) {
00804                 Vnm_print(2, "Valist_readXML: Unexpected token (%s) while \
00805 reading charge!\n", tok);
00806                 return VRC_FAILURE;
00807             }
00808             charge = dtmp;
00809             chgset = 1;
00810         } else if (Vstring_strcasecmp(tok, "radius") == 0) {
00811             Vio_scanf(sock, "%s", tok);
00812             if (sscanf(tok, "%lf", &dtmp) != 1) {
00813                 Vnm_print(2, "Valist_readXML: Unexpected token (%s) while \
00814 reading radius!\n", tok);
00815                 return VRC_FAILURE;
00816             }
00817             radius = dtmp;
00818             radset = 1;
00819         } else if (Vstring_strcasecmp(tok, "/atom") == 0) {
00820
00821             /* Get pointer to next available atom position */
00822             nextAtom = Valist_getAtomStorage(thee, &atoms, &nlist, &natoms);
00823             if (nextAtom == VNULL) {
00824                 Vnm_print(2, "Valist_readXML: Error in allocating spacing for atoms!\n");
00825                 return VRC_FAILURE;
00826             }
00827
00828             if (xset && yset && zset && chgset && radset){
00829
00830                 /* Store the information */
00831                 pos[0] = x; pos[1] = y; pos[2] = z;
00832                 Vatom_setPosition(nextAtom, pos);
00833                 Vatom_setCharge(nextAtom, charge);
00834                 Vatom_setRadius(nextAtom, radius);
00835                 Vatom_setAtomID(nextAtom, natoms-1);
00836
00837                 /* Reset the necessary flags */
00838                 xset = 0;
00839                 yset = 0;
00840                 zset = 0;
00841                 chgset = 0;
00842                 radset = 0;

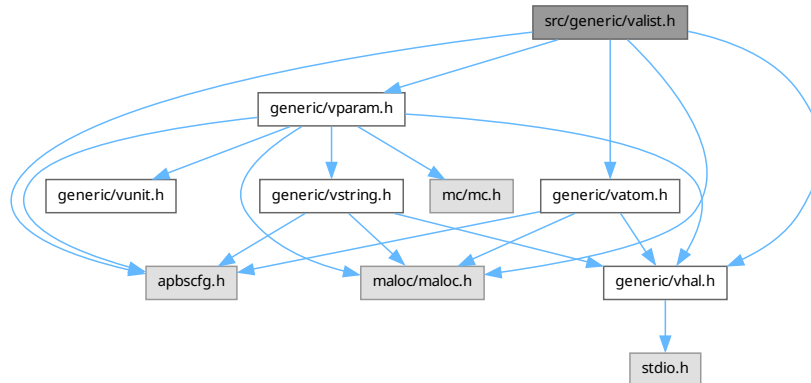
```

```
00843         } else {
00844             Vnm_print(2, "Valist_readXML: Missing field(s) in atom tag:\n");
00845             if (!xset) Vnm_print(2, "\tx value not set!\n");
00846             if (!yset) Vnm_print(2, "\ty value not set!\n");
00847             if (!zset) Vnm_print(2, "\tz value not set!\n");
00848             if (!chgset) Vnm_print(2, "\tcharge value not set!\n");
00849             if (!radset) Vnm_print(2, "\tradius value not set!\n");
00850             return VRC_FAILURE;
00851         }
00852     } else if (Vstring_strcasecmp(tok, endtag) == 0) break;
00853 }
00854
00855 Vnm_print(0, "Valist_readXML: Counted %d atoms\n", natoms);
00856 fflush(stdout);
00857
00858 /* Store atoms internally */
00859 if (Valist_setAtomArray(thee, &atoms, nlist, natoms) == VRC_FAILURE) {
00860     Vnm_print(2, "Valist_readXML: unable to store atoms!\n");
00861     return VRC_FAILURE;
00862 }
00863
00864 return Valist_getStatistics(thee);
00865
00866 }
00867
00868 /* Load up Valist with various statistics */
00869 VPUBLIC Vrc_Codes Valist_getStatistics(Valist *thee) {
00870     Vatom *atom;
00871     int i, j;
00872
00873     if (thee == VNULL) {
00874         Vnm_print(2, "Valist_getStatistics: Got NULL pointer when loading up Valist with various
00875 statistics!\n");
00876         VASSERT(0);
00877     }
00878
00879     thee->center[0] = 0.;
00880     thee->center[1] = 0.;
00881     thee->center[2] = 0.;
00882     thee->maxrad = 0.;
00883     thee->charge = 0.;
00884
00885     if (thee->number == 0) return VRC_FAILURE;
00886
00887     /* Reset stat variables */
00888     atom = &(thee->atoms[0]);
00889     for (i=0; i<3; i++) {
00890         thee->maxcrd[i] = thee->mincrd[i] = atom->position[i];
00891     }
00892     thee->maxrad = atom->radius;
00893     thee->charge = 0.0;
00894
00895     for (i=0; i<thee->number; i++) {
00896
00897         atom = &(thee->atoms[i]);
00898         for (j=0; j<3; j++) {
00899             if (atom->position[j] < thee->mincrd[j])
00900                 thee->mincrd[j] = atom->position[j];
00901             if (atom->position[j] > thee->maxcrd[j])
00902                 thee->maxcrd[j] = atom->position[j];
00903         }
00904         if (atom->radius > thee->maxrad) thee->maxrad = atom->radius;
00905         thee->charge = thee->charge + atom->charge;
00906     }
00907
00908     thee->center[0] = 0.5*(thee->maxcrd[0] + thee->mincrd[0]);
00909     thee->center[1] = 0.5*(thee->maxcrd[1] + thee->mincrd[1]);
00910     thee->center[2] = 0.5*(thee->maxcrd[2] + thee->mincrd[2]);
00911
00912     Vnm_print(0, "Valist_getStatistics: Max atom coordinate: (%g, %g, %g)\n",
00913               thee->maxcrd[0], thee->maxcrd[1], thee->maxcrd[2]);
00914     Vnm_print(0, "Valist_getStatistics: Min atom coordinate: (%g, %g, %g)\n",
00915               thee->mincrd[0], thee->mincrd[1], thee->mincrd[2]);
00916     Vnm_print(0, "Valist_getStatistics: Molecule center: (%g, %g, %g)\n",
00917               thee->center[0], thee->center[1], thee->center[2]);
00918
00919     return VRC_SUCCESS;
00920 }
```

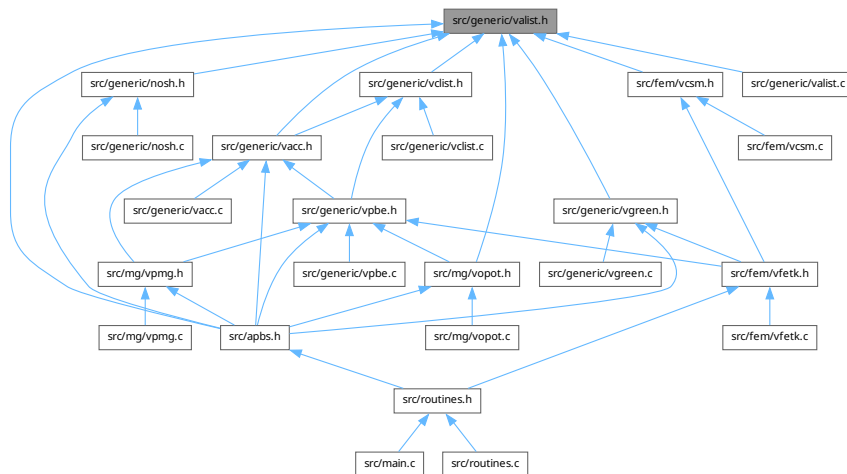
9.56 src/generic/valist.h File Reference

Contains declarations for class Valist.

```
#include "apbscfg.h"
#include "maloc/maloc.h"
#include "generic/vhal.h"
#include "generic/vatom.h"
#include "generic/vparam.h"
Include dependency graph for valist.h:
```



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [sValist](#)

Container class for list of atom objects.

Typedefs

- typedef struct [sValist](#) [Valist](#)

Declaration of the Valist class as the Valist structure.

Functions

- VEXTERNC [Vatom](#) * [Valist_getAtomList](#) ([Valist](#) *thee)
Get actual array of atom objects from the list.
- VEXTERNC double [Valist_getCenterX](#) ([Valist](#) *thee)
Get x-coordinate of molecule center.
- VEXTERNC double [Valist_getCenterY](#) ([Valist](#) *thee)
Get y-coordinate of molecule center.
- VEXTERNC double [Valist_getCenterZ](#) ([Valist](#) *thee)
Get z-coordinate of molecule center.
- VEXTERNC int [Valist_getNumberAtoms](#) ([Valist](#) *thee)
Get number of atoms in the list.
- VEXTERNC [Vatom](#) * [Valist_getAtom](#) ([Valist](#) *thee, int i)
Get pointer to particular atom in list.
- VEXTERNC unsigned long int [Valist_memChk](#) ([Valist](#) *thee)
Get total memory allocated for this object and its members.
- VEXTERNC [Valist](#) * [Valist_ctor](#) ()
Construct the atom list object.
- VEXTERNC [Vrc_Codes](#) [Valist_ctor2](#) ([Valist](#) *thee)
FORTTRAN stub to construct the atom list object.
- VEXTERNC void [Valist_dtor](#) ([Valist](#) **thee)
Destroys atom list object.
- VEXTERNC void [Valist_dtor2](#) ([Valist](#) *thee)
FORTTRAN stub to destroy atom list object.
- VEXTERNC [Vrc_Codes](#) [Valist_readPQR](#) ([Valist](#) *thee, [Vparam](#) *param, [Vio](#) *sock)
Fill atom list with information from a PQR file.
- VEXTERNC [Vrc_Codes](#) [Valist_readPDB](#) ([Valist](#) *thee, [Vparam](#) *param, [Vio](#) *sock)
Fill atom list with information from a PDB file.
- VEXTERNC [Vrc_Codes](#) [Valist_readXML](#) ([Valist](#) *thee, [Vparam](#) *param, [Vio](#) *sock)
Fill atom list with information from an XML file.
- VEXTERNC [Vrc_Codes](#) [Valist_getStatistics](#) ([Valist](#) *thee)
Load up Valist with various statistics.

9.56.1 Detailed Description

Contains declarations for class Valist.

Version

\$Id\$

Author

Nathan A. Baker

Attention

```

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*
*

```

Definition in file [valist.h](#).

9.57 valist.h

[Go to the documentation of this file.](#)

```

00001
00062 #ifndef _VALIST_H_
00063 #define _VALIST_H_
00064
00065 #include "apbscfg.h"
00066
00067 #include "malloc/malloc.h"
00068
00069 #include "generic/vhal.h"
00070 #include "generic/vatom.h"
00071 #include "generic/vparam.h"
00072
00078 struct sValist {
00079
00080     int number;

```

```

00081 double center[3];
00082 double mincrd[3];
00083 double maxcrd[3];
00084 double maxrad;
00085 double charge;
00086 Vatom *atoms;
00087 Vmem *vmem;
00089 };
00090
00095 typedef struct sValist Valist;
00096
00097 #if !defined(VINLINE_VATOM)
00098
00105 VEXTERNC Vatom* Valist_getAtomList(
00106     Valist *thee
00107 );
00108
00114 VEXTERNC double Valist_getCenterX(
00115     Valist *thee
00116 );
00117
00123 VEXTERNC double Valist_getCenterY(
00124     Valist *thee
00125 );
00126
00132 VEXTERNC double Valist_getCenterZ(
00133     Valist *thee
00134 );
00135
00141 VEXTERNC int Valist_getNumberAtoms(
00142     Valist *thee
00143 );
00144
00150 VEXTERNC Vatom* Valist_getAtom(
00151     Valist *thee,
00152     int i
00153 );
00154
00160 VEXTERNC unsigned long int Valist_memChk(
00161     Valist *thee
00162 );
00163
00164 #else /* if defined(VINLINE_VATOM) */
00165 # define Valist_getAtomList(thee) ((thee)->atoms)
00166 # define Valist_getNumberAtoms(thee) ((thee)->number)
00167 # define Valist_getAtom(thee, i) (&((thee)->atoms[i]))
00168 # define Valist_memChk(thee) (Vmem_bytes((thee)->vmem))
00169 # define Valist_getCenterX(thee) ((thee)->center[0])
00170 # define Valist_getCenterY(thee) ((thee)->center[1])
00171 # define Valist_getCenterZ(thee) ((thee)->center[2])
00172 #endif /* if !defined(VINLINE_VATOM) */
00173
00179 VEXTERNC Valist* Valist_ctor();
00180
00186 VEXTERNC Vrc_Codes Valist_ctor2(
00187     Valist *thee
00188 );
00189
00194 VEXTERNC void Valist_dtor(
00195     Valist **thee
00196 );
00197
00202 VEXTERNC void Valist_dtor2(
00203     Valist *thee
00204 );
00205
00217 VEXTERNC Vrc_Codes Valist_readPQR(
00218     Valist *thee,
00219     Vparam *param,
00220     Vio *sock
00221 );
00222
00232 VEXTERNC Vrc_Codes Valist_readPDB(
00233     Valist *thee,
00234     Vparam *param,
00235     Vio *sock
00236 );
00237
00247 VEXTERNC Vrc_Codes Valist_readXML(
00248     Valist *thee,
00249     Vparam *param,

```

```

00250         Vio *sock
00251     );
00252
00259 VEXTERNC Vrc_Codes Valist_getStatistics (Valist *thee);
00260
00261
00262 #endif /* ifndef _VALIST_H_ */

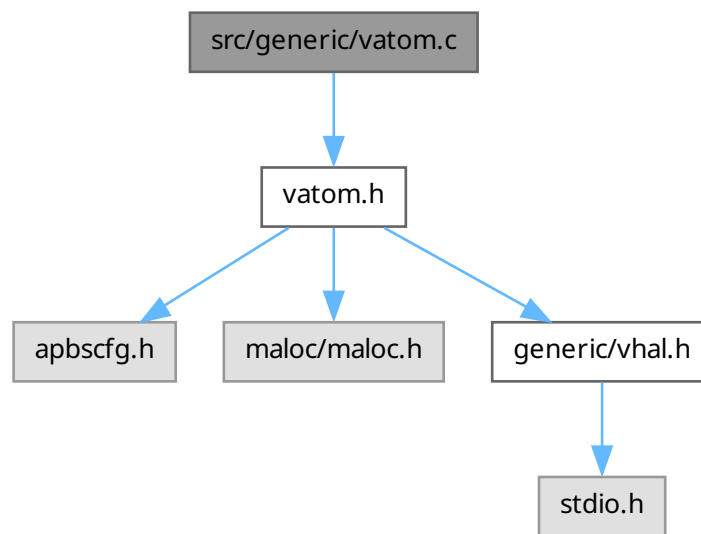
```

9.58 src/generic/vatom.c File Reference

Class Vatom methods.

```
#include "vatom.h"
```

Include dependency graph for vatom.c:



Functions

- VPUBLIC double * [Vatom_getPosition](#) ([Vatom](#) *thee)
Get atomic position.
- VPUBLIC double [Vatom_getPartID](#) ([Vatom](#) *thee)
Get partition ID.
- VPUBLIC void [Vatom_setPartID](#) ([Vatom](#) *thee, int partID)
Set partition ID.
- VPUBLIC double [Vatom_getAtomID](#) ([Vatom](#) *thee)
Get atom ID.
- VPUBLIC void [Vatom_setAtomID](#) ([Vatom](#) *thee, int atomID)
Set atom ID.
- VPUBLIC void [Vatom_setRadius](#) ([Vatom](#) *thee, double radius)
Set atomic radius.
- VPUBLIC double [Vatom_getRadius](#) ([Vatom](#) *thee)

- Get atomic position.*
- VPUBLIC void [Vatom_setCharge](#) ([Vatom](#) *thee, double charge)
- Set atomic charge.*
- VPUBLIC double [Vatom_getCharge](#) ([Vatom](#) *thee)
- Get atomic charge.*
- VPUBLIC void [Vatom_setEpsilon](#) ([Vatom](#) *thee, double epsilon)
- Set atomic epsilon.*
- VPUBLIC double [Vatom_getEpsilon](#) ([Vatom](#) *thee)
- Get atomic epsilon.*
- VPUBLIC unsigned long int [Vatom_memChk](#) ([Vatom](#) *thee)
- Return the memory used by this structure (and its contents) in bytes.*
- VPUBLIC [Vatom](#) * [Vatom_ctor](#) ()
- Constructor for the Vatom class.*
- VPUBLIC int [Vatom_ctor2](#) ([Vatom](#) *thee)
- FORTRAN stub constructor for the Vatom class.*
- VPUBLIC void [Vatom_dtor](#) ([Vatom](#) **thee)
- Object destructor.*
- VPUBLIC void [Vatom_dtor2](#) ([Vatom](#) *thee)
- FORTRAN stub object destructor.*
- VPUBLIC void [Vatom_setPosition](#) ([Vatom](#) *thee, double position[3])
- Set the atomic position.*
- VPUBLIC void [Vatom_copyTo](#) ([Vatom](#) *thee, [Vatom](#) *dest)
- Copy information to another atom.*
- VPUBLIC void [Vatom_copyFrom](#) ([Vatom](#) *thee, [Vatom](#) *src)
- Copy information to another atom.*
- VPUBLIC void [Vatom_setResName](#) ([Vatom](#) *thee, char resName[[VMAX_RECLEN](#)])
- Set residue name.*
- VPUBLIC void [Vatom_getResName](#) ([Vatom](#) *thee, char resName[[VMAX_RECLEN](#)])
- Retrieve residue name.*
- VPUBLIC void [Vatom_setAtomName](#) ([Vatom](#) *thee, char atomName[[VMAX_RECLEN](#)])
- Set atom name.*
- VPUBLIC void [Vatom_getAtomName](#) ([Vatom](#) *thee, char atomName[[VMAX_RECLEN](#)])
- Retrieve atom name.*

9.58.1 Detailed Description

Class Vatom methods.

Author

Nathan Baker

Version

\$Id\$

Attention

```

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*
*

```

Definition in file [vatom.c](#).

9.59 vatom.c

[Go to the documentation of this file.](#)

```

00001
00057 #include "vatom.h"
00058
00059 VEMBED(rcsid="$Id$")
00060
00061 #if !defined(VINLINE_VATOM)
00062
00063 VPUBLIC double *Vatom_getPosition(Vatom *thee) {
00064
00065     VASSERT(thee != VNULL);
00066     return thee->position;
00067 }
00068
00069
00070 VPUBLIC double Vatom_getPartID(Vatom *thee) {

```

```

00071
00072     VASSERT(thee != VNULL);
00073     return thee->partID;
00074
00075 }
00076
00077 VPUBLIC void Vatom_setPartID(Vatom *thee, int partID) {
00078
00079     VASSERT(thee != VNULL);
00080     thee->partID = (double)partID;
00081
00082 }
00083
00084 VPUBLIC double Vatom_getAtomID(Vatom *thee) {
00085
00086     VASSERT(thee != VNULL);
00087     return thee->id;
00088
00089 }
00090
00091 VPUBLIC void Vatom_setAtomID(Vatom *thee, int atomID) {
00092
00093     VASSERT(thee != VNULL);
00094     thee->id = atomID;
00095
00096 }
00097
00098 VPUBLIC void Vatom_setRadius(Vatom *thee, double radius) {
00099
00100     VASSERT(thee != VNULL);
00101     thee->radius = radius;
00102
00103 }
00104
00105 VPUBLIC double Vatom_getRadius(Vatom *thee) {
00106
00107     VASSERT(thee != VNULL);
00108     return thee->radius;
00109
00110 }
00111
00112 VPUBLIC void Vatom_setCharge(Vatom *thee, double charge) {
00113
00114     VASSERT(thee != VNULL);
00115     thee->charge = charge;
00116
00117 }
00118
00119 VPUBLIC double Vatom_getCharge(Vatom *thee) {
00120
00121     VASSERT(thee != VNULL);
00122     return thee->charge;
00123
00124 }
00125
00126 VPUBLIC void Vatom_setEpsilon(Vatom *thee, double epsilon) {
00127
00128     VASSERT(thee != VNULL);
00129     thee->epsilon = epsilon;
00130
00131 }
00132 VPUBLIC double Vatom_getEpsilon(Vatom *thee) {
00133
00134     VASSERT(thee != VNULL);
00135     return thee->epsilon;
00136 }
00137
00138 VPUBLIC unsigned long int Vatom_memChk(Vatom *thee) { return sizeof(Vatom); }
00139
00140 #endif /* if !defined(VINLINE_VATOM) */
00141
00142 VPUBLIC Vatom* Vatom_ctor() {
00143
00144     /* Set up the structure */
00145     Vatom *thee = VNULL;
00146     thee = (Vatom *)Vmem_malloc( VNULL, 1, sizeof(Vatom) );
00147     VASSERT( thee != VNULL);
00148     VASSERT( Vatom_ctor2(thee));
00149
00150     return thee;
00151 }

```

```

00152
00153 VPUBLIC int Vatom_ctor2(Vatom *thee) {
00154     thee->partID = -1;
00155     return 1;
00156 }
00157
00158 VPUBLIC void Vatom_dtor(Vatom **thee) {
00159     if ((*thee) != VNULL) {
00160         Vatom_dtor2(*thee);
00161         Vmem_free(VNULL, 1, sizeof(Vatom), (void **)thee);
00162         (*thee) = VNULL;
00163     }
00164 }
00165
00166 VPUBLIC void Vatom_dtor2(Vatom *thee) { ; }
00167
00168 VPUBLIC void Vatom_setPosition(Vatom *thee, double position[3]) {
00169
00170     VASSERT(thee != VNULL);
00171     (thee->position)[0] = position[0];
00172     (thee->position)[1] = position[1];
00173     (thee->position)[2] = position[2];
00174
00175 }
00176
00177 VPUBLIC void Vatom_copyTo(Vatom *thee, Vatom *dest) {
00178
00179     VASSERT(thee != VNULL);
00180     VASSERT(dest != VNULL);
00181
00182     memcpy(dest, thee, sizeof(Vatom));
00183
00184 }
00185
00186 VPUBLIC void Vatom_copyFrom(Vatom *thee, Vatom *src) {
00187
00188     Vatom_copyTo(src, thee);
00189
00190 }
00191
00192 VPUBLIC void Vatom_setResName(Vatom *thee, char resName[VMAX_RECLEN]) {
00193
00194     VASSERT(thee != VNULL);
00195     strcpy(thee->resName, resName);
00196
00197 }
00198
00199 VPUBLIC void Vatom_getResName(Vatom *thee, char resName[VMAX_RECLEN]) {
00200
00201
00202     VASSERT(thee != VNULL);
00203     strcpy(resName, thee->resName);
00204
00205 }
00206
00207 VPUBLIC void Vatom_setAtomName(Vatom *thee, char atomName[VMAX_RECLEN]) {
00208
00209     VASSERT(thee != VNULL);
00210     strcpy(thee->atomName, atomName);
00211
00212 }
00213
00214 VPUBLIC void Vatom_getAtomName(Vatom *thee, char atomName[VMAX_RECLEN]) {
00215
00216     VASSERT(thee != VNULL);
00217     strcpy(atomName, thee->atomName);
00218
00219 }
00220
00221 #if defined(WITH_TINKER)
00222
00223 VPUBLIC void Vatom_setDipole(Vatom *thee, double dipole[3]) {
00224
00225     VASSERT(thee != VNULL);
00226     (thee->dipole)[0] = dipole[0];
00227     (thee->dipole)[1] = dipole[1];
00228     (thee->dipole)[2] = dipole[2];
00229
00230 }
00231
00232 VPUBLIC void Vatom_setQuadrupole(Vatom *thee, double quadrupole[9]) {

```



```

00233
00234     int i;
00235     VASSERT(thee != VNULL);
00236     for (i=0; i<9; i++) (thee->quadrupole)[i] = quadrupole[i];
00237 }
00238
00239 VPUBLIC void Vatom_setInducedDipole(Vatom *thee, double dipole[3]) {
00240
00241     VASSERT(thee != VNULL);
00242     (thee->inducedDipole)[0] = dipole[0];
00243     (thee->inducedDipole)[1] = dipole[1];
00244     (thee->inducedDipole)[2] = dipole[2];
00245 }
00246
00247 VPUBLIC void Vatom_setNLInducedDipole(Vatom *thee, double dipole[3]) {
00248
00249     VASSERT(thee != VNULL);
00250     (thee->nlInducedDipole)[0] = dipole[0];
00251     (thee->nlInducedDipole)[1] = dipole[1];
00252     (thee->nlInducedDipole)[2] = dipole[2];
00253 }
00254 }
00255
00256 VPUBLIC double *Vatom_getDipole(Vatom *thee) {
00257
00258     VASSERT(thee != VNULL);
00259     return thee->dipole;
00260 }
00261 }
00262
00263 VPUBLIC double *Vatom_getQuadrupole(Vatom *thee) {
00264
00265     VASSERT(thee != VNULL);
00266     return thee->quadrupole;
00267 }
00268 }
00269
00270 VPUBLIC double *Vatom_getInducedDipole(Vatom *thee) {
00271
00272     VASSERT(thee != VNULL);
00273     return thee->inducedDipole;
00274 }
00275 }
00276
00277 VPUBLIC double *Vatom_getNLInducedDipole(Vatom *thee) {
00278
00279     VASSERT(thee != VNULL);
00280     return thee->nlInducedDipole;
00281 }
00282 }
00283
00284 #endif /* if defined(WITH_TINKER) */

```

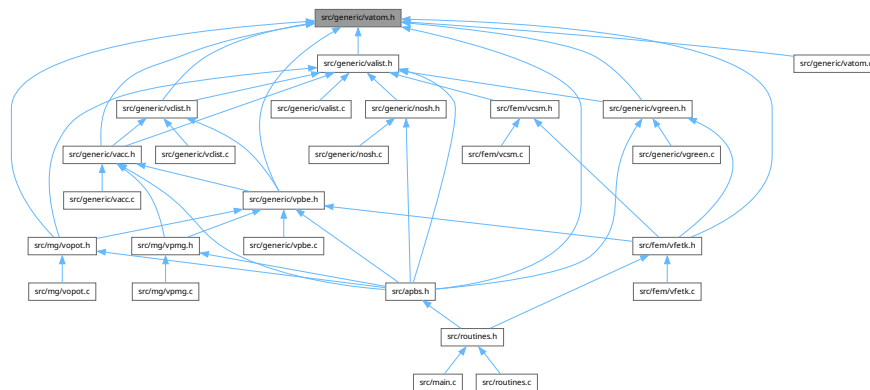
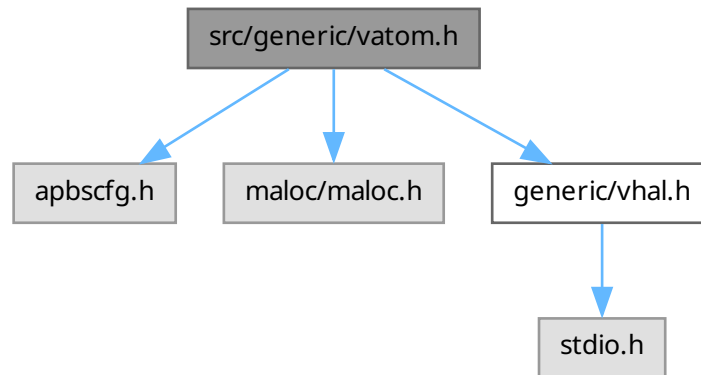
9.60 src/generic/vatom.h File Reference

Contains declarations for class Vatom.

```

#include "apbscfg.h"
#include "malloc/malloc.h"
#include "generic/vhal.h"

```



- struct sVatom

- Contains public data members for Vatom class/module.*

- #define VMAX_RECLEN 64

- Residue name length.*

- typedef struct sVatom Vatom

- Declaration of the Vatom class as the Vatom structure.*

Functions

- VEXTERNC double * [Vatom_getPosition](#) ([Vatom](#) *thee)
Get atomic position.
- VEXTERNC void [Vatom_setRadius](#) ([Vatom](#) *thee, double radius)
Set atomic radius.
- VEXTERNC double [Vatom_getRadius](#) ([Vatom](#) *thee)
Get atomic position.
- VEXTERNC void [Vatom_setPartID](#) ([Vatom](#) *thee, int partID)
Set partition ID.
- VEXTERNC double [Vatom_getPartID](#) ([Vatom](#) *thee)
Get partition ID.
- VEXTERNC void [Vatom_setAtomID](#) ([Vatom](#) *thee, int id)
Set atom ID.
- VEXTERNC double [Vatom_getAtomID](#) ([Vatom](#) *thee)
Get atom ID.
- VEXTERNC void [Vatom_setCharge](#) ([Vatom](#) *thee, double charge)
Set atomic charge.
- VEXTERNC double [Vatom_getCharge](#) ([Vatom](#) *thee)
Get atomic charge.
- VEXTERNC void [Vatom_setEpsilon](#) ([Vatom](#) *thee, double epsilon)
Set atomic epsilon.
- VEXTERNC double [Vatom_getEpsilon](#) ([Vatom](#) *thee)
Get atomic epsilon.
- VEXTERNC unsigned long int [Vatom_memChk](#) ([Vatom](#) *thee)
Return the memory used by this structure (and its contents) in bytes.
- VEXTERNC void [Vatom_setResName](#) ([Vatom](#) *thee, char resName[VMAX_RECLEN])
Set residue name.
- VEXTERNC void [Vatom_setAtomName](#) ([Vatom](#) *thee, char atomName[VMAX_RECLEN])
Set atom name.
- VEXTERNC void [Vatom_getResName](#) ([Vatom](#) *thee, char resName[VMAX_RECLEN])
Retrieve residue name.
- VEXTERNC void [Vatom_getAtomName](#) ([Vatom](#) *thee, char atomName[VMAX_RECLEN])
Retrieve atom name.
- VEXTERNC [Vatom](#) * [Vatom_ctor](#) ()
Constructor for the Vatom class.
- VEXTERNC int [Vatom_ctor2](#) ([Vatom](#) *thee)
FORTTRAN stub constructor for the Vatom class.
- VEXTERNC void [Vatom_dtor](#) ([Vatom](#) **thee)
Object destructor.
- VEXTERNC void [Vatom_dtor2](#) ([Vatom](#) *thee)
FORTTRAN stub object destructor.
- VEXTERNC void [Vatom_setPosition](#) ([Vatom](#) *thee, double position[3])
Set the atomic position.
- VEXTERNC void [Vatom_copyTo](#) ([Vatom](#) *thee, [Vatom](#) *dest)
Copy information to another atom.
- VEXTERNC void [Vatom_copyFrom](#) ([Vatom](#) *thee, [Vatom](#) *src)
Copy information to another atom.

9.60.1 Detailed Description

Contains declarations for class Vatom.

Version

\$Id\$

Author

Nathan A. Baker

Attention

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*
```

Definition in file [vatom.h](#).

9.61 vatom.h

[Go to the documentation of this file.](#)

```

00001
00062 #ifndef _VATOM_H_
00063 #define _VATOM_H_
00064
00065 #include "apbscfg.h"
00066
00067 #include "malloc/malloc.h"
00068
00069 #include "generic/vhal.h"
00070
00077 #define VMAX_RECLEN      64
00078
00084 struct sVatom {
00085     double position[3];
00086     double radius;
00087     double charge;
00088     double partID;
00091     double epsilon;
00093     int id;
00097     char resName[VMAX_RECLEN];
00098     char atomName[VMAX_RECLEN];
00100 #if defined(WITH_TINKER)
00101
00102     double dipole[3];
00103     double quadrupole[9];
00104     double inducedDipole[3];
00105     double nlInducedDipole[3];
00107 #endif /* if defined(WITH_TINKER) */
00108 };
00109
00114 typedef struct sVatom Vatom;
00115
00116 #if !defined(VINLINE_VATOM)
00117
00124 VEXTERNC double* Vatom_getPosition(Vatom *thee);
00125
00132 VEXTERNC void Vatom_setRadius(Vatom *thee, double radius);
00133
00140 VEXTERNC double Vatom_getRadius(Vatom *thee);
00141
00149 VEXTERNC void Vatom_setPartID(Vatom *thee, int partID);
00150
00158 VEXTERNC double Vatom_getPartID(Vatom *thee);
00159
00166 VEXTERNC void Vatom_setAtomID(Vatom *thee, int id);
00167
00174 VEXTERNC double Vatom_getAtomID(Vatom *thee);
00175
00182 VEXTERNC void Vatom_setCharge(Vatom *thee, double charge);
00183
00190 VEXTERNC double Vatom_getCharge(Vatom *thee);
00191
00198 VEXTERNC void Vatom_setEpsilon(Vatom *thee, double epsilon);
00199
00206 VEXTERNC double Vatom_getEpsilon(Vatom *thee);
00207
00215 VEXTERNC unsigned long int Vatom_memChk(Vatom *thee);
00216
00217 #else /* if defined(VINLINE_VATOM) */
00218 # define Vatom_getPosition(thee) ((thee)->position)
00219 # define Vatom_setRadius(thee, tRadius) ((thee)->radius = (tRadius))
00220 # define Vatom_getRadius(thee) ((thee)->radius)
00221 # define Vatom_setPartID(thee, tpartID) ((thee)->partID = (double)(tpartID))
00222 # define Vatom_getPartID(thee) ((thee)->partID)
00223 # define Vatom_setAtomID(thee, tatomID) ((thee)->id = (tatomID))
00224 # define Vatom_getAtomID(thee) ((thee)->id)
00225 # define Vatom_setCharge(thee, tCharge) ((thee)->charge = (tCharge))
00226 # define Vatom_getCharge(thee) ((thee)->charge)
00227 # define Vatom_setEpsilon(thee, tEpsilon) ((thee)->epsilon = (tEpsilon))
00228 # define Vatom_getEpsilon(thee) ((thee)->epsilon)
00229 # define Vatom_memChk(thee) (sizeof(Vatom))
00230 #endif /* if !defined(VINLINE_VATOM) */
00231
00232 /* ////////////////////////////////////// */
00233 // Class Vatom: Non-Inlineable methods (vatom.c)
00235
00242 VEXTERNC void Vatom_setResName(Vatom *thee, char resName[VMAX_RECLEN]);
00243
00248 VEXTERNC void Vatom_setAtomName(
00249     Vatom *thee, /**< Vatom object */

```

```

00250         char atomName[VMAX_RECLEN]
00251     );
00252
00259 VEXTERNC void    Vatom_getResName(Vatom *thee, char resName[VMAX_RECLEN]);
00260
00265 VEXTERNC void    Vatom_getAtomName(
00266     Vatom *thee,
00267     char atomName[VMAX_RECLEN]
00268 );
00269
00275 VEXTERNC Vatom* Vatom_ctor();
00276
00283 VEXTERNC int     Vatom_ctor2(Vatom *thee);
00284
00290 VEXTERNC void    Vatom_dtor(Vatom **thee);
00291
00297 VEXTERNC void    Vatom_dtor2(Vatom *thee);
00298
00305 VEXTERNC void    Vatom_setPosition(Vatom *thee, double position[3]);
00306
00314 VEXTERNC void    Vatom_copyTo(Vatom *thee, Vatom *dest);
00315
00323 VEXTERNC void    Vatom_copyFrom(Vatom *thee, Vatom *src);
00324
00325 #if defined(WITH_TINKER)
00326
00333 VEXTERNC void    Vatom_setInducedDipole(Vatom *thee,
00334                                         double inducedDipole[3]);
00335
00342 VEXTERNC void    Vatom_setNLInducedDipole(Vatom *thee,
00343                                             double nlInducedDipole[3]);
00344
00351 VEXTERNC void    Vatom_setDipole(Vatom *thee, double dipole[3]);
00352
00359 VEXTERNC void    Vatom_setQuadrupole(Vatom *thee, double quadrupole[9]);
00360
00366 VEXTERNC double* Vatom_getDipole(Vatom *thee);
00367
00373 VEXTERNC double* Vatom_getQuadrupole(Vatom *thee);
00374
00380 VEXTERNC double* Vatom_getInducedDipole(Vatom *thee);
00381
00387 VEXTERNC double* Vatom_getNLInducedDipole(Vatom *thee);
00388 #endif /* if defined(WITH_TINKER) */
00389
00390 #endif /* ifndef _VATOM_H_ */

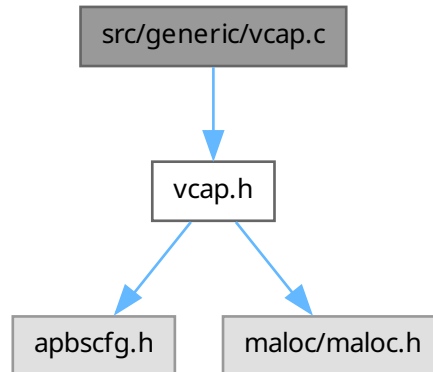
```

9.62 src/generic/vcap.c File Reference

Class Vcap methods.

```
#include "vcap.h"
```

Include dependency graph for vcap.c:



Functions

- VPUBLIC double [Vcap_exp](#) (double x, int *ichop)
Provide a capped exp() function.
- VPUBLIC double [Vcap_sinh](#) (double x, int *ichop)
Provide a capped sinh() function.
- VPUBLIC double [Vcap_cosh](#) (double x, int *ichop)
Provide a capped cosh() function.

9.62.1 Detailed Description

Class Vcap methods.

Author

Nathan Baker

Version

\$Id\$

Attention

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*
*

```

Definition in file [vcap.c](#).

9.63 vcap.c

[Go to the documentation of this file.](#)

```

00001
00057 #include "vcap.h"
00058
00059 VPUBLIC double Vcap_exp(double x, int *ichop) {
00060
00061     /* The two chopped arguments */
00062     if (x > EXPMAX) {
00063         (*ichop) = 1;
00064         return VEXP(EXPMAX);
00065     } else if (x < EXPMIN) {
00066         (*ichop) = 1;
00067         return VEXP(EXPMIN);
00068     }
00069
00070     /* The normal EXP */
00071     (*ichop) = 0;
00072     return VEXP(x);
00073 }
00074
00075 VPUBLIC double Vcap_sinh(double x, int *ichop) {
00076
00077     /* The two chopped arguments */
00078     if (x > EXPMAX) {
00079         (*ichop) = 1;
00080         return VSINH(EXPMAX);
00081     } else if (x < EXPMIN) {
00082         (*ichop) = 1;
00083         return VSINH(EXPMIN);
00084     }
00085

```



```
00086      /* The normal SINH */
00087      (*ichop) = 0;
00088      return VSINH(x);
00089  }
00090
00091  VPUBLIC double Vcap_cosh(double x, int *ichop) {
00092
00093      /* The two chopped arguments */
00094      if (x > EXPMAX) {
00095          (*ichop) = 1;
00096          return VCOSH(EXPMAX);
00097      } else if (x < EXPMIN) {
00098          (*ichop) = 1;
00099          return VCOSH(EXPMIN);
00100      }
00101
00102      /* The normal COSH */
00103      (*ichop) = 0;
00104      return VCOSH(x);
00105  }
```

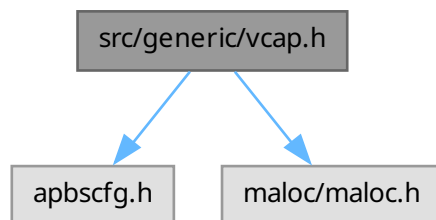
9.64 src/generic/vcap.h File Reference

Contains declarations for class Vcap.

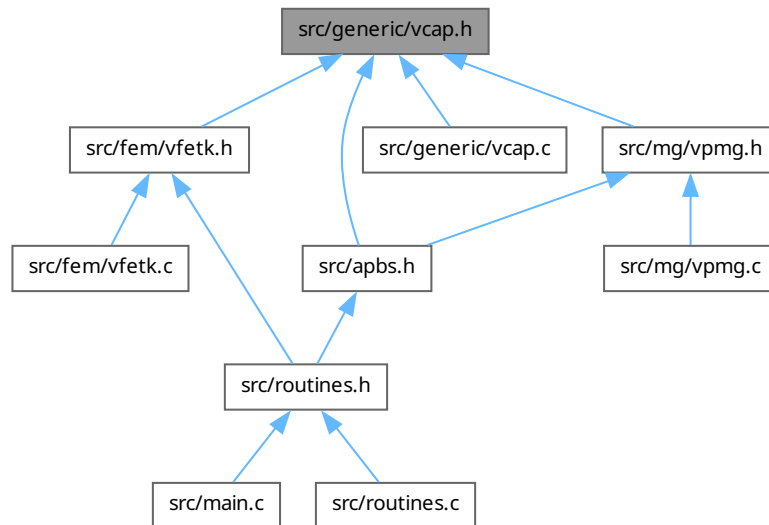
```
#include "apbscfg.h"
```

```
#include "maloc/maloc.h"
```

Include dependency graph for vcap.h:



This graph shows which files directly or indirectly include this file:



Macros

- #define **EXPMAX** 85.00
Maximum argument for exp(), sinh(), or cosh()
- #define **EXPMIN** -85.00
Minimum argument for exp(), sinh(), or cosh()

Functions

- VEXTERNC double **Vcap_exp** (double x, int *ichop)
Provide a capped exp() function.
- VEXTERNC double **Vcap_sinh** (double x, int *ichop)
Provide a capped sinh() function.
- VEXTERNC double **Vcap_cosh** (double x, int *ichop)
Provide a capped cosh() function.

9.64.1 Detailed Description

Contains declarations for class Vcap.

Version

\$Id\$

Author

Nathan A. Baker

Attention

```

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```

Definition in file [vcap.h](#).

9.65 vcap.h

[Go to the documentation of this file.](#)

```

00001
00064 #ifndef _VCAP_H_
00065 #define _VCAP_H_
00066
00067 #include "apbscfg.h"
00068
00072 #define EXPMAX 85.00
00073
00077 #define EXPMIN -85.00
00078
00079 #include "maloc/maloc.h"
00080
00099 VEXTERNC double Vcap_exp(
00100     double x,
00101     int *ichop

```

```

00102         );
00103
00104
00123 VEXTERNC double Vcap_sinh(
00124     double x,
00125     int *ichop
00126 );
00127
00146 VEXTERNC double Vcap_cosh(
00147     double x,
00148     int *ichop
00149 );
00150
00151 #endif /* ifndef _VCAP_H_ */

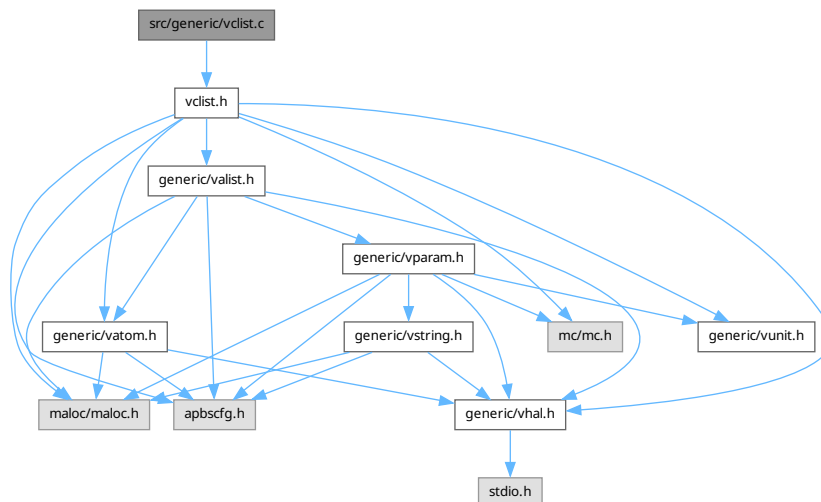
```

9.66 src/generic/vclist.c File Reference

Class Vclist methods.

```
#include "vclist.h"
```

Include dependency graph for vclist.c:



Macros

- #define **VCLIST_INFLATE** 1.42

Functions

- VPUBLIC unsigned long int **Vclist_memChk** (Vclist *thee)
Get number of bytes in this object and its members.
- VPUBLIC double **Vclist_maxRadius** (Vclist *thee)
Get the max probe radius value (in Å) the cell list was constructed with.
- VPUBLIC Vclist * **Vclist_ctor** (Valist *alist, double max_radius, int npts[VAPBS_DIM], Vclist_DomainMode mode, double lower_corner[VAPBS_DIM], double upper_corner[VAPBS_DIM])
Construct the cell list object.
- VPRIVATE void **Vclist_getMolDims** (Vclist *thee, double lower_corner[VAPBS_DIM], double upper_↵
corner[VAPBS_DIM], double *r_max)

- VPRIVATE Vrc_Codes [Vclist_setupGrid](#) ([Vclist](#) *thee)
- VPRIVATE Vrc_Codes [Vclist_storeParms](#) ([Vclist](#) *thee, [Valist](#) *alist, double max_radius, int npts[[VAPBS_DIM](#)], [Vclist_DomainMode](#) mode, double lower_corner[[VAPBS_DIM](#)], double upper_corner[[VAPBS_DIM](#)])
- VPRIVATE void [Vclist_gridSpan](#) ([Vclist](#) *thee, [Vatom](#) *atom, int imin[[VAPBS_DIM](#)], int imax[[VAPBS_DIM](#)])
- VPRIVATE int [Vclist_arrayIndex](#) ([Vclist](#) *thee, int i, int j, int k)
- VPRIVATE Vrc_Codes [Vclist_assignAtoms](#) ([Vclist](#) *thee)
- VPUBLIC Vrc_Codes [Vclist_ctor2](#) ([Vclist](#) *thee, [Valist](#) *alist, double max_radius, int npts[[VAPBS_DIM](#)], [Vclist_DomainMode](#) mode, double lower_corner[[VAPBS_DIM](#)], double upper_corner[[VAPBS_DIM](#)])
FORTTRAN stub to construct the cell list object.
- VPUBLIC void [Vclist_dtor](#) ([Vclist](#) **thee)
Destroy object.
- VPUBLIC void [Vclist_dtor2](#) ([Vclist](#) *thee)
FORTTRAN stub to destroy object.
- VPUBLIC [VclistCell](#) * [Vclist_getCell](#) ([Vclist](#) *thee, double pos[[VAPBS_DIM](#)])
Return cell corresponding to specified position or return VNULL.
- VPUBLIC [VclistCell](#) * [VclistCell_ctor](#) (int natoms)
Allocate and construct a cell list cell object.
- VPUBLIC Vrc_Codes [VclistCell_ctor2](#) ([VclistCell](#) *thee, int natoms)
Construct a cell list object.
- VPUBLIC void [VclistCell_dtor](#) ([VclistCell](#) **thee)
Destroy object.
- VPUBLIC void [VclistCell_dtor2](#) ([VclistCell](#) *thee)
FORTTRAN stub to destroy object.

9.66.1 Detailed Description

Class Vclist methods.

Author

Nathan Baker

Version

\$Id\$

Attention

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*

```

Definition in file [vclist.c](#).

9.66.2 Function Documentation

9.66.2.1 Vclist_arrayIndex()

```

VPRIVATE int Vclist_arrayIndex (
    Vclist * thee,
    int i,
    int j,
    int k )

```

Definition at line 262 of file [vclist.c](#).

9.66.2.2 Vclist_assignAtoms()

```

VPRIVATE Vrc_Codes Vclist_assignAtoms (
    Vclist * thee )

```

Definition at line 270 of file [vclist.c](#).

9.66.2.3 Vclist_getMolDims()

```

VPRIVATE void Vclist_getMolDims (
    Vclist * thee,
    double lower_corner[VAPBS_DIM],
    double upper_corner[VAPBS_DIM],
    double * r_max )

```

Definition at line 90 of file [vclist.c](#).

9.66.2.4 Vclist_gridSpan()

```

VPRIVATE void Vclist_gridSpan (
    Vclist * thee,
    Vatom * atom,

```

```

    int imin[VAPBS_DIM],
    int imax[VAPBS_DIM] )

```

Definition at line 231 of file [vclist.c](#).

9.66.2.5 Vclist_setupGrid()

```

VPRIVATE Vrc_Codes Vclist_setupGrid (
    Vclist * thee )

```

Definition at line 125 of file [vclist.c](#).

9.66.2.6 Vclist_storeParms()

```

VPRIVATE Vrc_Codes Vclist_storeParms (
    Vclist * thee,
    Valist * alist,
    double max_radius,
    int npts[VAPBS_DIM],
    Vclist_DomainMode mode,
    double lower_corner[VAPBS_DIM],
    double upper_corner[VAPBS_DIM] )

```

Definition at line 174 of file [vclist.c](#).

9.67 vclist.c

[Go to the documentation of this file.](#)

```

00001
00057 #include "vclist.h"
00058
00059 VEMBED(rcsid="$Id$")
00060
00061 #if !defined(VINLINE_VCLIST)
00062
00063 VPUBLIC unsigned long int Vclist_memChk(Vclist *thee) {
00064     if (thee == VNULL) return 0;
00065     return Vmem_bytes(thee->vmem);
00066 }
00067
00068 VPUBLIC double Vclist_maxRadius(Vclist *thee) {
00069     VASSERT(thee != VNULL);
00070     return thee->max_radius;
00071 }
00072
00073 #endif /* if !defined(VINLINE_VCLIST) */
00074
00075 VPUBLIC Vclist* Vclist_ctor(Valist *alist, double max_radius,
00076     int npts[VAPBS_DIM], Vclist_DomainMode mode,
00077     double lower_corner[VAPBS_DIM], double upper_corner[VAPBS_DIM]) {
00078
00079     Vclist *thee = VNULL;
00080
00081     /* Set up the structure */
00082     thee = (Vclist*)Vmem_malloc(VNULL, 1, sizeof(Vclist) );
00083     VASSERT( thee != VNULL);
00084     VASSERT( Vclist_ctor2(thee, alist, max_radius, npts, mode, lower_corner,
00085         upper_corner) == VRC_SUCCESS );
00086     return thee;
00087 }
00088
00089 /* Get the dimensions of the molecule stored in thee->alist */
00090 VPRIVATE void Vclist_getMolDims(
00091     Vclist *thee,
00092     double lower_corner[VAPBS_DIM], /* Set to lower corner of molecule */
00093     double upper_corner[VAPBS_DIM], /* Set to lower corner of molecule */
00094     double *r_max /* Set to max atom radius */
00095 ) {
00096
00097     int i, j;
00098     double pos;

```

```

00099     Valist *alist;
00100     Vatom *atom;
00101
00102     alist = thee->alist;
00103
00104     /* Initialize */
00105     for (i=0; i<VAPBS_DIM; i++) {
00106         lower_corner[i] = VLARGE;
00107         upper_corner[i] = -VLARGE;
00108     }
00109     *r_max = -1.0;
00110
00111     /* Check each atom */
00112     for (i=0; i<Valist_getNumberAtoms(alist); i++) {
00113         atom = Valist_getAtom(alist, i);
00114         for (j=0; j<VAPBS_DIM; j++) {
00115             pos = (Vatom_getPosition(atom))[j];
00116             if ( pos < lower_corner[j] ) lower_corner[j] = pos;
00117             if ( pos > upper_corner[j] ) upper_corner[j] = pos;
00118         }
00119         if (Vatom_getRadius(atom) > *r_max) *r_max = Vatom_getRadius(atom);
00120     }
00121 }
00122 }
00123
00124 /* Setup lookup grid */
00125 VPRIVATE Vrc_Codes Vclist_setupGrid(Vclist *thee) {
00126
00127     /* Inflation factor ~ sqrt(2)*/
00128     #define VCLIST_INFLATE 1.42
00129
00130     int i;
00131     double length[VAPBS_DIM], r_max;
00132
00133     /* Set up the grid corners */
00134     switch (thee->mode) {
00135         case CLIST_AUTO_DOMAIN:
00136             /* Get molecule dimensions */
00137             Vclist_getMolDims(thee, thee->lower_corner, thee->upper_corner,
00138                             &r_max);
00139             /* Set up grid spacings */
00140             for (i=0; i<VAPBS_DIM; i++) {
00141                 thee->upper_corner[i] = thee->upper_corner[i]
00142                     + VCLIST_INFLATE*(r_max+thee->max_radius);
00143                 thee->lower_corner[i] = thee->lower_corner[i]
00144                     - VCLIST_INFLATE*(r_max+thee->max_radius);
00145             }
00146             break;
00147         case CLIST_MANUAL_DOMAIN:
00148             /* Grid corners established in constructor */
00149             break;
00150         default:
00151             Vnm_print(2, "Vclist_setupGrid: invalid setup mode (%d)!\n",
00152                     thee->mode);
00153             return VRC_FAILURE;
00154     }
00155
00156     /* Set up the grid lengths and spacings */
00157     for (i=0; i<VAPBS_DIM; i++) {
00158         length[i] = thee->upper_corner[i] - thee->lower_corner[i];
00159         thee->spacs[i] = length[i]/((double)(thee->npts[i] - 1));
00160     }
00161     Vnm_print(0, "Vclist_setupGrid: Grid lengths = (%g, %g, %g)\n",
00162             length[0], length[1], length[2]);
00163
00164     Vnm_print(0, "Vclist_setupGrid: Grid lower corner = (%g, %g, %g)\n",
00165             (thee->lower_corner)[0], (thee->lower_corner)[1],
00166             (thee->lower_corner)[2]);
00167
00168     return VRC_SUCCESS;
00169
00170     #undef VCLIST_INFLATE
00171 }
00172
00173 /* Check and store parameters passed to constructor */
00174 VPRIVATE Vrc_Codes Vclist_storeParms(Vclist *thee, Valist *alist,
00175     double max_radius, int npts[VAPBS_DIM], Vclist_DomainMode mode,
00176     double lower_corner[VAPBS_DIM], double upper_corner[VAPBS_DIM] ) {
00177
00178     int i = 0;
00179

```



```

00180     if (alist == VNULL) {
00181         Vnm_print(2, "Vclist_ctor2: Got NULL Valist!\n");
00182         return VRC_FAILURE;
00183     } else thee->alist = alist;
00184
00185     thee->n = 1;
00186     for (i=0; i<VAPBS_DIM; i++) {
00187         if (npts[i] < 3) {
00188             Vnm_print(2,
00189                 "Vclist_ctor2: n[%d] (%d) must be greater than 2!\n",
00190                 i, npts[i]);
00191             return VRC_FAILURE;
00192         }
00193         thee->npts[i] = npts[i];
00194         thee->n *= npts[i];
00195     }
00196     Vnm_print(0, "Vclist_ctor2: Using %d x %d x %d hash table\n",
00197         npts[0], npts[1], npts[2]);
00198
00199     thee->mode = mode;
00200     switch (thee->mode) {
00201     case CLIST_AUTO_DOMAIN:
00202         Vnm_print(0, "Vclist_ctor2: automatic domain setup.\n");
00203         break;
00204     case CLIST_MANUAL_DOMAIN:
00205         Vnm_print(0, "Vclist_ctor2: manual domain setup.\n");
00206         Vnm_print(0, "Vclist_ctor2: lower corner = [ \n");
00207         for (i=0; i<VAPBS_DIM; i++) {
00208             thee->lower_corner[i] = lower_corner[i];
00209             Vnm_print(0, "%g ", lower_corner[i]);
00210         }
00211         Vnm_print(0, "]\n");
00212         Vnm_print(0, "Vclist_ctor2: upper corner = [ \n");
00213         for (i=0; i<VAPBS_DIM; i++) {
00214             thee->upper_corner[i] = upper_corner[i];
00215             Vnm_print(0, "%g ", upper_corner[i]);
00216         }
00217         Vnm_print(0, "]\n");
00218         break;
00219     default:
00220         Vnm_print(2, "Vclist_ctor2: invalid setup mode (%d)!\n", mode);
00221         return VRC_FAILURE;
00222     }
00223
00224     thee->max_radius = max_radius;
00225     Vnm_print(0, "Vclist_ctor2: Using %g max radius\n", max_radius);
00226
00227     return VRC_SUCCESS;
00228 }
00229
00230 /* Calculate the gridpoints an atom spans */
00231 VPRIVATE void Vclist_gridSpan(Vclist *thee,
00232     Vatom *atom, /* Atom */
00233     int imin[VAPBS_DIM], /* Set to min grid indices */
00234     int imax[VAPBS_DIM] /* Set to max grid indices */
00235 ) {
00236
00237     int i;
00238     double *coord, dc, idc, rtot;
00239
00240     /* Get the position in the grid's frame of reference */
00241     coord = Vatom_getPosition(atom);
00242
00243     /* Get the range the atom radius + probe radius spans */
00244     rtot = Vatom_getRadius(atom) + thee->max_radius;
00245
00246     /* Calculate the range of grid points the inflated atom spans in the x
00247     * direction. */
00248     for (i=0; i<VAPBS_DIM; i++) {
00249         dc = coord[i] - (thee->lower_corner)[i];
00250         idc = (dc + rtot)/(thee->spacs[i]);
00251         imax[i] = (int)(ceil(idc));
00252         imax[i] = VMIN2(imax[i], thee->npts[i]-1);
00253         idc = (dc - rtot)/(thee->spacs[i]);
00254         imin[i] = (int)(floor(idc));
00255         imin[i] = VMAX2(imin[i], 0);
00256     }
00257
00258 }
00259
00260 /* Get the array index for a particular cell based on its i,j,k

```

```

00261  * coordinates */
00262  VPRIVATE int Vclist_arrayIndex(Vclist *thee, int i, int j, int k) {
00263
00264      return (thee->npts[2])*(thee->npts[1])*i + (thee->npts[2])*j + k;
00265
00266  }
00267
00268
00269  /* Assign atoms to cells */
00270  VPRIVATE Vrc_Codes Vclist_assignAtoms(Vclist *thee) {
00271
00272      int iatom, i, j, k, ui, inext;
00273      int imax[VAPBS_DIM], imin[VAPBS_DIM];
00274      int totatoms;
00275      Vatom *atom;
00276      VclistCell *cell;
00277
00278
00279      /* Find out how many atoms are associated with each grid point */
00280      totatoms = 0;
00281      for (iatom=0; iatom<Valist_getNumberAtoms(thee->alist); iatom++) {
00282
00283          /* Get grid span for atom */
00284          atom = Valist_getAtom(thee->alist, iatom);
00285          Vclist_gridSpan(thee, atom, imin, imax);
00286
00287          /* Now find and assign the grid points */
00288          VASSERT(VAPBS_DIM == 3);
00289          for (i = imin[0]; i <= imax[0]; i++) {
00290              for (j = imin[1]; j <= imax[1]; j++) {
00291                  for (k = imin[2]; k <= imax[2]; k++) {
00292                      /* Get index to array */
00293                      ui = Vclist_arrayIndex(thee, i, j, k);
00294                      /* Increment number of atoms for this grid point */
00295                      cell = &(thee->cells[ui]);
00296                      (cell->natoms)++;
00297                      totatoms++;
00298                  }
00299              }
00300          }
00301      }
00302      Vnm_print(0, "Vclist_assignAtoms: Have %d atom entries\n", totatoms);
00303
00304      /* Allocate the space to store the pointers to the atoms */
00305      for (ui=0; ui<thee->n; ui++) {
00306          cell = &(thee->cells[ui]);
00307          if ( VclistCell_ctor2(cell, cell->natoms) == VRC_FAILURE ) {
00308              Vnm_print(2, "Vclist_assignAtoms: cell error!\n");
00309              return VRC_FAILURE;
00310          }
00311          /* Clear the counter for later use */
00312          cell->natoms = 0;
00313      }
00314
00315      /* Assign the atoms to grid points */
00316      for (iatom=0; iatom<Valist_getNumberAtoms(thee->alist); iatom++) {
00317
00318          /* Get grid span for atom */
00319          atom = Valist_getAtom(thee->alist, iatom);
00320          Vclist_gridSpan(thee, atom, imin, imax);
00321
00322          /* Now find and assign the grid points */
00323          for (i = imin[0]; i <= imax[0]; i++) {
00324              for (j = imin[1]; j <= imax[1]; j++) {
00325                  for (k = imin[2]; k <= imax[2]; k++) {
00326                      /* Get index to array */
00327                      ui = Vclist_arrayIndex(thee, i, j, k);
00328                      cell = &(thee->cells[ui]);
00329                      /* Index of next available array location */
00330                      inext = cell->natoms;
00331                      cell->atoms[inext] = atom;
00332                      /* Increment number of atoms */
00333                      (cell->natoms)++;
00334                  }
00335              }
00336          }
00337      }
00338
00339      return VRC_SUCCESS;
00340  }
00341

```

```

00342 /* Main (FORTRAN stub) constructor */
00343 VPUBLIC Vrc_Codes Vclist_ctor2(Vclist *thee, Valist *alist, double max_radius,
00344     int npts[VAPBS_DIM], Vclist_DomainMode mode,
00345     double lower_corner[VAPBS_DIM], double upper_corner[VAPBS_DIM]) {
00346
00347     int i;
00348     VclistCell *cell;
00349
00350     /* Check and store parameters */
00351     if ( Vclist_storeParms(thee, alist, max_radius, npts, mode, lower_corner,
00352         upper_corner) == VRC_FAILURE ) {
00353         Vnm_print(2, "Vclist_ctor2:  parameter check failed!\n");
00354         return VRC_FAILURE;
00355     }
00356
00357     /* Set up memory */
00358     thee->vmem = Vmem_ctor("APBS::VCLIST");
00359     if (thee->vmem == VNULL) {
00360         Vnm_print(2, "Vclist_ctor2:  memory object setup failed!\n");
00361         return VRC_FAILURE;
00362     }
00363
00364     /* Set up cells */
00365     thee->cells = (VclistCell*)Vmem_malloc( thee->vmem, thee->n, sizeof(VclistCell) );
00366     if (thee->cells == VNULL) {
00367         Vnm_print(2,
00368             "Vclist_ctor2:  Failed allocating %d VclistCell objects!\n",
00369             thee->n);
00370         return VRC_FAILURE;
00371     }
00372     for (i=0; i<thee->n; i++) {
00373         cell = &(thee->cells[i]);
00374         cell->natoms = 0;
00375     }
00376
00377     /* Set up the grid */
00378     if ( Vclist_setupGrid(thee) == VRC_FAILURE ) {
00379         Vnm_print(2, "Vclist_ctor2:  grid setup failed!\n");
00380         return VRC_FAILURE;
00381     }
00382
00383     /* Assign atoms to grid cells */
00384     if (Vclist_assignAtoms(thee) == VRC_FAILURE) {
00385         Vnm_print(2, "Vclist_ctor2:  atom assignment failed!\n");
00386         return VRC_FAILURE;
00387     }
00388
00389
00390
00391
00392
00393     return VRC_SUCCESS;
00394 }
00395
00396 /* Destructor */
00397 VPUBLIC void Vclist_dtor(Vclist **thee) {
00398
00399     if ((*thee) != VNULL) {
00400         Vclist_dtor2(*thee);
00401         Vmem_free(VNULL, 1, sizeof(Vclist), (void **)thee);
00402         (*thee) = VNULL;
00403     }
00404
00405 }
00406
00407 /* Main (stub) destructor */
00408 VPUBLIC void Vclist_dtor2(Vclist *thee) {
00409
00410     VclistCell *cell;
00411     int i;
00412
00413     for (i=0; i<thee->n; i++) {
00414         cell = &(thee->cells[i]);
00415         VclistCell_dtor2(cell);
00416     }
00417     Vmem_free(thee->vmem, thee->n, sizeof(VclistCell),
00418         (void **)&(thee->cells));
00419     Vmem_dtor(&(thee->vmem));
00420
00421 }
00422

```

```

00423 VPUBLIC VclistCell* Vclist_getCell(Vclist *thee,
00424                                     double pos[VAPBS_DIM]
00425                                     ) {
00426
00427     int i,
00428         ic[VAPBS_DIM],
00429         ui;
00430     double c[VAPBS_DIM];
00431
00432     /* Assert this before we do anything else, since its failure should fail the function */
00433     VASSERT(VAPBS_DIM == 3);
00434
00435     /* Convert to grid based coordinates */
00436     for (i=0; i<VAPBS_DIM; i++) {
00437         c[i] = pos[i] - (thee->lower_corner)[i];
00438         ic[i] = (int)(c[i]/thee->spacs[i]);
00439
00440         if (ic[i] < 0 || ic[i] >= thee->npts[i]) {
00441             return VNULL;
00442         }
00443     }
00444
00445     /* Get the array index */
00446     ui = Vclist_arrayIndex(thee, ic[0], ic[1], ic[2]);
00447
00448     return &(thee->cells[ui]);
00449 }
00450
00451 VPUBLIC VclistCell* VclistCell_ctor(int natoms) {
00452     VclistCell *thee = VNULL;
00453
00454     /* Set up the structure */
00455     thee = (VclistCell*)Vmem_malloc(VNULL, 1, sizeof(VclistCell));
00456     VASSERT( thee != VNULL);
00457     VASSERT( VclistCell_ctor2(thee, natoms) == VRC_SUCCESS );
00458
00459     return thee;
00460 }
00461
00462 VPUBLIC Vrc_Codes VclistCell_ctor2(VclistCell *thee, int natoms) {
00463     if (thee == VNULL) {
00464         Vnm_print(2, "VclistCell_ctor2: NULL thee!\n");
00465         return VRC_FAILURE;
00466     }
00467
00468     thee->natoms = natoms;
00469     if (thee->natoms > 0) {
00470         thee->atoms = (Vatom**)Vmem_malloc(VNULL, natoms, sizeof(Vatom *));
00471         if (thee->atoms == VNULL) {
00472             Vnm_print(2,
00473                 "VclistCell_ctor2: unable to allocate space for %d atom pointers!\n",
00474                 natoms);
00475             return VRC_FAILURE;
00476         }
00477     }
00478
00479     return VRC_SUCCESS;
00480 }
00481
00482 VPUBLIC void VclistCell_dtor(VclistCell **thee) {
00483     if ((*thee) != VNULL) {
00484         VclistCell_dtor2(*thee);
00485         Vmem_free(VNULL, 1, sizeof(VclistCell), (void **)thee);
00486         (*thee) = VNULL;
00487     }
00488 }
00489
00490 /* Main (stub) destructor */
00491 VPUBLIC void VclistCell_dtor2(VclistCell *thee) {
00492     if (thee->natoms > 0) {
00493         Vmem_free(VNULL, thee->natoms, sizeof(Vatom *),
00494             (void **)&(thee->atoms));
00495     }
00496 }

```

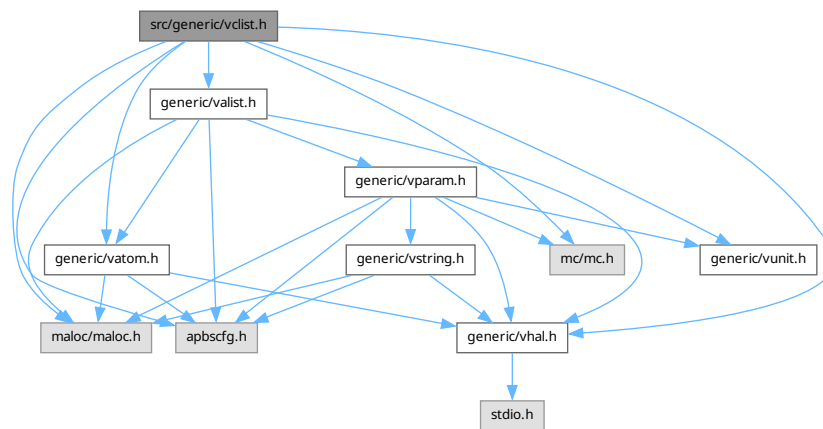
```
00504 }
```

9.68 src/generic/vclist.h File Reference

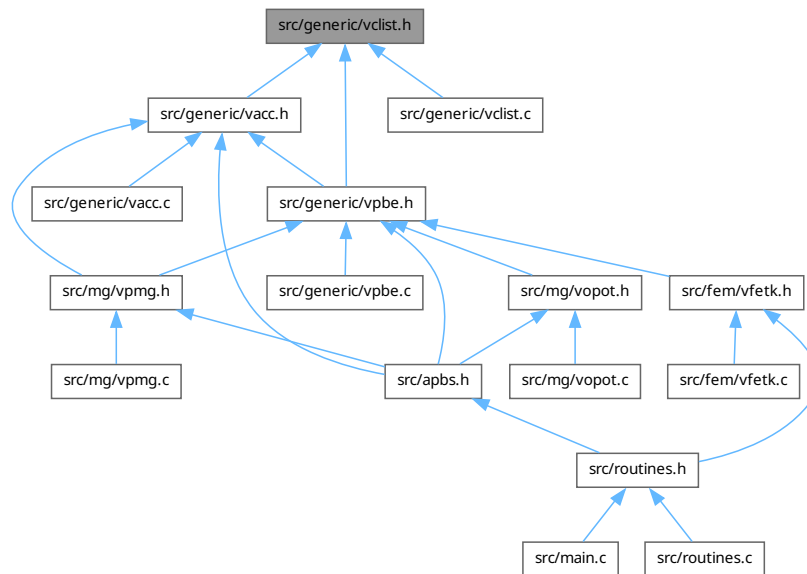
Contains declarations for class Vclist.

```
#include "apbscfg.h"
#include "maloc/maloc.h"
#include "mc/mc.h"
#include "generic/vhal.h"
#include "generic/valist.h"
#include "generic/vatom.h"
#include "generic/vunit.h"
```

Include dependency graph for vclist.h:



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [sVclistCell](#)
Atom cell list cell.
- struct [sVclist](#)
Atom cell list.

Typedefs

- typedef enum [eVclist_DomainMode](#) [Vclist_DomainMode](#)
- typedef struct [sVclistCell](#) [VclistCell](#)
Declaration of the VclistCell class as the VclistCell structure.
- typedef struct [sVclist](#) [Vclist](#)
Declaration of the Vclist class as the Vclist structure.

Enumerations

- enum [eVclist_DomainMode](#) { [CLIST_AUTO_DOMAIN](#) , [CLIST_MANUAL_DOMAIN](#) }
Atom cell list domain setup mode.

Functions

- VEXTERNC unsigned long int [Vclist_memChk](#) ([Vclist](#) *thee)
Get number of bytes in this object and its members.
- VEXTERNC double [Vclist_maxRadius](#) ([Vclist](#) *thee)
Get the max probe radius value (in Å) the cell list was constructed with.

- VEXTERNC `Vclist * Vclist_ctor (Valist *alist, double max_radius, int npts[VAPBS_DIM], Vclist_DomainMode mode, double lower_corner[VAPBS_DIM], double upper_corner[VAPBS_DIM])`
Construct the cell list object.
- VEXTERNC `Vrc_Codes Vclist_ctor2 (Vclist *thee, Valist *alist, double max_radius, int npts[VAPBS_DIM], Vclist_DomainMode mode, double lower_corner[VAPBS_DIM], double upper_corner[VAPBS_DIM])`
FORTTRAN stub to construct the cell list object.
- VEXTERNC `void Vclist_dtor (Vclist **thee)`
Destroy object.
- VEXTERNC `void Vclist_dtor2 (Vclist *thee)`
FORTTRAN stub to destroy object.
- VEXTERNC `VclistCell * Vclist_getCell (Vclist *thee, double position[VAPBS_DIM])`
Return cell corresponding to specified position or return VNULL.
- VEXTERNC `VclistCell * VclistCell_ctor (int natoms)`
Allocate and construct a cell list cell object.
- VEXTERNC `Vrc_Codes VclistCell_ctor2 (VclistCell *thee, int natoms)`
Construct a cell list object.
- VEXTERNC `void VclistCell_dtor (VclistCell **thee)`
Destroy object.
- VEXTERNC `void VclistCell_dtor2 (VclistCell *thee)`
FORTTRAN stub to destroy object.

9.68.1 Detailed Description

Contains declarations for class Vclist.

Version

\$Id\$

Author

Nathan A. Baker

Attention

```
*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
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* Pacific Northwest National Laboratory
*
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* THE POSSIBILITY OF SUCH DAMAGE.
*
*

```

Definition in file [vclist.h](#).

9.68.2 Typedef Documentation

9.68.2.1 Vclist_DomainMode

```
typedef enum eVclist_DomainMode Vclist_DomainMode
```

Definition at line 94 of file [vclist.h](#).

9.69 vclist.h

[Go to the documentation of this file.](#)

```

00001
00062 #ifndef _VCLIST_H_
00063 #define _VCLIST_H_
00064
00065 #include "apbscfg.h"
00066
00067 #include "malloc/malloc.h"
00068 #if defined(HAVE_MC_H)
00069 #include "mc/mc.h"
00070 #endif
00071
00072 #include "generic/vhal.h"
00073 #include "generic/valist.h"
00074 #include "generic/vatom.h"
00075 #include "generic/vunit.h"
00076
00082 enum eVclist_DomainMode {
00083     CLIST_AUTO_DOMAIN,
00085     CLIST_MANUAL_DOMAIN
00087 };
00088
00094 typedef enum eVclist_DomainMode Vclist_DomainMode;
00095
00101 struct sVclistCell {
00102     Vatom **atoms;
00103     int natoms;
00104 };
00105
00110 typedef struct sVclistCell VclistCell;
00111
00117 struct sVclist {
00118
00119     Vmem *vmem;
00120     Valist *alist;

```



```

00121  Vclist_DomainMode mode;
00122  int npts[VAPBS_DIM];
00123  int n;
00124  double max_radius;
00125  VclistCell *cells;
00126  double lower_corner[VAPBS_DIM];
00127  double upper_corner[VAPBS_DIM];
00128  double spacs[VAPBS_DIM];
00130 };
00131
00136 typedef struct sVclist Vclist;
00137
00138 #if !defined(VINLINE_VCLIST)
00139
00145  VEXTERNC unsigned long int Vclist_memChk(
00146      Vclist *thee
00147  );
00148
00156  VEXTERNC double Vclist_maxRadius(
00157      Vclist *thee
00158  );
00159
00160 #else /* if defined(VINLINE_VCLIST) */
00161
00162 #   define Vclist_memChk(thee) (Vmem_bytes((thee)->vmem))
00163 #   define Vclist_maxRadius(thee) ((thee)->max_radius)
00164
00165 #endif /* if !defined(VINLINE_VCLIST) */
00166
00167 /* ////////////////////////////////////// */
00168 // Class Vclist: Non-Inlineable methods (vclist.c)
00170
00175 VEXTERNC Vclist* Vclist_ctor(
00176     Valist *alist, /**< Molecule for cell list queries */
00177     double max_radius,
00178     int npts[VAPBS_DIM],
00180     Vclist_DomainMode mode,
00181     double lower_corner[VAPBS_DIM],
00184     double upper_corner[VAPBS_DIM]
00187 );
00188
00193 VEXTERNC Vrc_Codes Vclist_ctor2(
00194     Vclist *thee,
00195     Valist *alist,
00196     double max_radius,
00197     int npts[VAPBS_DIM],
00199     Vclist_DomainMode mode,
00200     double lower_corner[VAPBS_DIM],
00203     double upper_corner[VAPBS_DIM]
00206 );
00207
00212 VEXTERNC void Vclist_dtor(
00213     Vclist **thee
00214 );
00215
00220 VEXTERNC void Vclist_dtor2(
00221     Vclist *thee
00222 );
00223
00231 VEXTERNC VclistCell* Vclist_getCell(
00232     Vclist *thee,
00233     double position[VAPBS_DIM]
00234 );
00235
00242 VEXTERNC VclistCell* VclistCell_ctor(
00243     int natoms
00244 );
00245
00252 VEXTERNC Vrc_Codes VclistCell_ctor2(
00253     VclistCell *thee,
00254     int natoms
00255 );
00256
00261 VEXTERNC void VclistCell_dtor(
00262     VclistCell **thee
00263 );
00264
00269 VEXTERNC void VclistCell_dtor2(
00270     VclistCell *thee
00271 );
00272

```

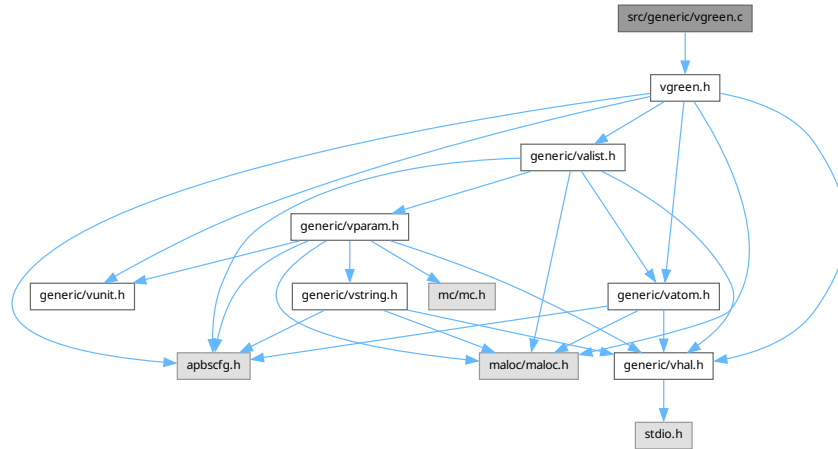
```
00273 #endif      /* ifndef _VCLIST_H_ */
```

9.70 src/generic/vgreen.c File Reference

Class Vgreen methods.

```
#include "vgreen.h"
```

Include dependency graph for vgreen.c:



Functions

- VPRIVATE int [treesetup](#) ([Vgreen](#) *thee)
- VPRIVATE int [treecleanup](#) ([Vgreen](#) *thee)
- VPRIVATE int [treecalc](#) ([Vgreen](#) *thee, double *xtar, double *ytar, double *ztar, double *qtar, int numtars, double *tpengtar, double *x, double *y, double *z, double *q, int numpars, double *fx, double *fy, double *fz, int iflag, int farrdim, int arrdim)
- VPUBLIC [Valist](#) * [Vgreen_getValist](#) ([Vgreen](#) *thee)

Get the atom list associated with this Green's function object.
- VPUBLIC unsigned long int [Vgreen_memChk](#) ([Vgreen](#) *thee)

Return the memory used by this structure (and its contents) in bytes.
- VPUBLIC [Vgreen](#) * [Vgreen_ctor](#) ([Valist](#) *alist)

Construct the Green's function oracle.
- VPUBLIC int [Vgreen_ctor2](#) ([Vgreen](#) *thee, [Valist](#) *alist)

FORTTRAN stub to construct the Green's function oracle.
- VPUBLIC void [Vgreen_dtor](#) ([Vgreen](#) **thee)

Destruct the Green's function oracle.
- VPUBLIC void [Vgreen_dtor2](#) ([Vgreen](#) *thee)

FORTTRAN stub to destruct the Green's function oracle.
- VPUBLIC int [Vgreen_helmholtz](#) ([Vgreen](#) *thee, int npos, double *x, double *y, double *z, double *val, double kappa)

Get the Green's function for Helmholtz's equation integrated over the atomic point charges.
- VPUBLIC int [Vgreen_helmholtzD](#) ([Vgreen](#) *thee, int npos, double *x, double *y, double *z, double *gradx, double *grady, double *gradz, double kappa)

Get the gradient of Green's function for Helmholtz's equation integrated over the atomic point charges.

- VPUBLIC int [Vgreen_coulomb_direct](#) ([Vgreen](#) *thee, int npos, double *x, double *y, double *z, double *val)

Get the Coulomb's Law Green's function (solution to Laplace's equation) integrated over the atomic point charges using direct summation.

- VPUBLIC int [Vgreen_coulomb](#) ([Vgreen](#) *thee, int npos, double *x, double *y, double *z, double *val)

Get the Coulomb's Law Green's function (solution to Laplace's equation) integrated over the atomic point charges using direct summation or H. E. Johnston, R. Krasny FMM library (if available)

- VPUBLIC int [Vgreen_coulombD_direct](#) ([Vgreen](#) *thee, int npos, double *x, double *y, double *z, double *pot, double *gradx, double *grady, double *gradz)

Get gradient of the Coulomb's Law Green's function (solution to Laplace's equation) integrated over the atomic point charges using direct summation.

- VPUBLIC int [Vgreen_coulombD](#) ([Vgreen](#) *thee, int npos, double *x, double *y, double *z, double *pot, double *gradx, double *grady, double *gradz)

Get gradient of the Coulomb's Law Green's function (solution to Laplace's equation) integrated over the atomic point charges using either direct summation or H. E. Johnston/R. Krasny FMM library (if available)

9.70.1 Detailed Description

Class Vgreen methods.

Author

Nathan Baker

Version

\$Id\$

Attention

```
*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
* Nathan A. Baker (nathan.baker@pnnl.gov)
* Pacific Northwest National Laboratory
*
* Additional contributing authors listed in the code documentation.
*
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* THE POSSIBILITY OF SUCH DAMAGE.
*
*

```

Definition in file [vgreen.c](#).

9.70.2 Function Documentation

9.70.2.1 treecalc()

```

VPRIVATE int treecalc (
    Vgreen * thee,
    double * xtar,
    double * ytar,
    double * ztar,
    double * qtar,
    int numtars,
    double * tpengtar,
    double * x,
    double * y,
    double * z,
    double * q,
    int numpars,
    double * fx,
    double * fy,
    double * fz,
    int iflag,
    int farrdim,
    int arrdim )

```

Definition at line 525 of file [vgreen.c](#).

9.70.2.2 treecleanup()

```

VPRIVATE int treecleanup (
    Vgreen * thee )

```

Definition at line 505 of file [vgreen.c](#).

9.70.2.3 treesetup()

```

VPRIVATE int treesetup (
    Vgreen * thee )

```

Definition at line 425 of file [vgreen.c](#).

9.71 vgreen.c

[Go to the documentation of this file.](#)

```

00001
00057 #include "vgreen.h"
00058
00059 /* Define wrappers for F77 treecode routines */
00060 #ifndef HAVE_TREE
00061 # define F77TREEPEFORCE VF77_MANGLE(treepeforce, TREEPEFORCE)
00062 # define F77DIRECT_ENG_FORCE VF77_MANGLE(direct_eng_force, DIRECT_ENG_FORCE)
00063 # define F77CLEANUP VF77_MANGLE(mycleanup, MYCLEANUP)
00064 # define F77TREE_COMP VF77_MANGLE(mytree_compp, MYTREE_COMP)
00065 # define F77TREE_COMPFP VF77_MANGLE(mytree_comppf, MYTREE_COMPFP)
00066 # define F77CREATE_TREE VF77_MANGLE(mycreate_tree, MYCREATE_TREE)
00067 # define F77INITLEVELS VF77_MANGLE(myinitlevels, MYINITLEVELS)
00068 # define F77SETUP VF77_MANGLE(mysetup, MYSETUP)
00069 #endif /* ifdef HAVE_TREE */
00070
00071 /* Some constants associated with the tree code */
00072 #ifndef HAVE_TREE
00076 # define FMM_DIST_TOL VSMALL
00082 # define FMM_IFLAG 2
00086 # define FMM_ORDER 4
00090 # define FMM_THETA 0.5
00094 # define FMM_MAXPARNODE 150
00098 # define FMM_SHRINK 1
00102 # define FMM_MINLEVEL 50000
00106 # define FMM_MAXLEVEL 0
00107 #endif /* ifdef HAVE_TREE */
00108
00109
00110 /*
00111  * @brief Setup treecode internal structures
00112  * @ingroup Vgreen
00113  * @author Nathan Baker
00114  * @param thee Vgreen object
00115  * @return 1 if successful, 0 otherwise
00116  */
00117 VPRIVATE int treesetup(Vgreen *thee);
00118
00119 /*
00120  * @brief Clean up treecode internal structures
00121  * @ingroup Vgreen
00122  * @author Nathan Baker
00123  * @param thee Vgreen object
00124  * @return 1 if successful, 0 otherwise
00125  */
00126 VPRIVATE int treecleanup(Vgreen *thee);
00127
00128 /*
00129  * @brief Calculate forces or potential
00130  * @ingroup Vgreen
00131  * @author Nathan Baker
00132  * @param thee Vgreen object
00133  * @return 1 if successful, 0 otherwise
00134  */
00135 VPRIVATE int treecalc(Vgreen *thee, double *xtar, double *ytar, double *ztar,
00136 double *qtar, int numtars, double *tpengtar, double *x, double *y,
00137 double *z, double *g, int numpars, double *fx, double *fy, double *fz,
00138 int iflag, int farrdim, int arddim);
00139
00140 #if !defined(VINLINE_VGREEN)
00141
00142 VPUBLIC Valist* Vgreen_getValist(Vgreen *thee) {
00143     VASSERT(thee != VNULL);
00144     return thee->alist;
00145 }
00146
00147 }
00148
00149 VPUBLIC unsigned long int Vgreen_memChk(Vgreen *thee) {
00150     if (thee == VNULL) return 0;
00151     return Vmem_bytes(thee->vmem);
00152 }
00153
00154 #endif /* if !defined(VINLINE_VGREEN) */
00155
00156 VPUBLIC Vgreen* Vgreen_ctor(Valist *alist) {
00157     /* Set up the structure */
00158     Vgreen *thee = VNULL;
00159     thee = (Vgreen *)Vmem_malloc(VNULL, 1, sizeof(Vgreen));
00160     VASSERT(thee != VNULL);
00161     VASSERT(Vgreen_ctor2(thee, alist));
00162

```

```

00163
00164     return thee;
00165 }
00166
00167 VPUBLIC int Vgreen_ctor2(Vgreen *thee, Valist *alist) {
00168
00169     VASSERT( thee != VNULL );
00170
00171     /* Memory management object */
00172     thee->vmem = Vmem_ctor("APBS:VGREEN");
00173
00174     /* Set up the atom list and grid manager */
00175     if (alist == VNULL) {
00176         Vnm_print(2, "Vgreen_ctor2: got null pointer to Valist object!\n");
00177     }
00178
00179     thee->alist = alist;
00180
00181     /* Setup FMM tree (if applicable) */
00182     #ifdef HAVE_TREE
00183     if (!treesetup(thee)) {
00184         Vnm_print(2, "Vgreen_ctor2: Error setting up FMM tree!\n");
00185         return 0;
00186     }
00187     #endif /* ifdef HAVE_TREE */
00188
00189     return 1;
00190 }
00191
00192 VPUBLIC void Vgreen_dtor(Vgreen **thee) {
00193     if ((*thee) != VNULL) {
00194         Vgreen_dtor2(*thee);
00195         Vmem_free(VNULL, 1, sizeof(Vgreen), (void **)thee);
00196         (*thee) = VNULL;
00197     }
00198 }
00199
00200 VPUBLIC void Vgreen_dtor2(Vgreen *thee) {
00201
00202     #ifdef HAVE_TREE
00203     treecleanup(thee);
00204     #endif
00205     Vmem_dtor(&(thee->vmem));
00206 }
00207
00208
00209 VPUBLIC int Vgreen_helmholtz(Vgreen *thee, int npos, double *x, double *y,
00210     double *z, double *val, double kappa) {
00211
00212     Vnm_print(2, "Error -- Vgreen_helmholtz not implemented yet!\n");
00213     return 0;
00214 }
00215
00216 VPUBLIC int Vgreen_helmholtzD(Vgreen *thee, int npos, double *x, double *y,
00217     double *z, double *gradx, double *grady, double *gradz, double kappa) {
00218
00219     Vnm_print(2, "Error -- Vgreen_helmholtzD not implemented yet!\n");
00220     return 0;
00221 }
00222
00223
00224 VPUBLIC int Vgreen_coulomb_direct(Vgreen *thee, int npos, double *x,
00225     double *y, double *z, double *val) {
00226
00227     Vatom *atom;
00228     double *apos, charge, dist, dx, dy, dz, scale;
00229     double *q, qtemp, fx, fy, fz;
00230     int iatom, ipos;
00231
00232     if (thee == VNULL) {
00233         Vnm_print(2, "Vgreen_coulomb: Got NULL thee!\n");
00234         return 0;
00235     }
00236
00237     for (ipos=0; ipos<npos; ipos++) val[ipos] = 0.0;
00238
00239     for (iatom=0; iatom<Valist_getNumberAtoms(thee->alist); iatom++) {
00240         atom = Valist_getAtom(thee->alist, iatom);
00241         apos = Vatom_getPosition(atom);
00242         charge = Vatom_getCharge(atom);
00243         for (ipos=0; ipos<npos; ipos++) {

```

```

00244         dx = apos[0] - x[ipos];
00245         dy = apos[1] - y[ipos];
00246         dz = apos[2] - z[ipos];
00247         dist = VSQRT(VSQR(dx) + VSQR(dy) + VSQR(dz));
00248         if (dist > VSMALL) val[ipos] += (charge/dist);
00249     }
00250 }
00251
00252     scale = Vunit_ec/(4*Vunit_pi*Vunit_eps0*1.0e-10);
00253     for (ipos=0; ipos<npos; ipos++) val[ipos] = val[ipos]*scale;
00254
00255     return 1;
00256 }
00257
00258 VPUBLIC int Vgreen_coulomb(Vgreen *thee, int npos, double *x, double *y,
00259     double *z, double *val) {
00260
00261     Vatom *atom;
00262     double *apos, charge, dist, dx, dy, dz, scale;
00263     double *q, qtemp, fx, fy, fz;
00264     int iatom, ipos;
00265
00266     if (thee == VNULL) {
00267         Vnm_print(2, "Vgreen_coulomb: Got NULL thee!\n");
00268         return 0;
00269     }
00270
00271     for (ipos=0; ipos<npos; ipos++) val[ipos] = 0.0;
00272
00273 #ifdef HAVE_TREE
00274
00275     /* Allocate charge array (if necessary) */
00276     if (Valist_getNumberAtoms(thee->alist) > 1) {
00277         if (npos > 1) {
00278             q = VNULL;
00279             q = Vmem_malloc(thee->vmem, npos, sizeof(double));
00280             if (q == VNULL) {
00281                 Vnm_print(2, "Vgreen_coulomb: Error allocating charge array!\n");
00282                 return 0;
00283             }
00284         } else {
00285             q = &(qtemp);
00286         }
00287         for (ipos=0; ipos<npos; ipos++) q[ipos] = 1.0;
00288
00289         /* Calculate */
00290         treecalc(thee, x, y, z, q, npos, val, thee->xp, thee->yp, thee->zp,
00291             thee->qp, thee->np, &fx, &fy, &fz, 1, 1, thee->np);
00292     } else return Vgreen_coulomb_direct(thee, npos, x, y, z, val);
00293
00294     /* De-allocate charge array (if necessary) */
00295     if (npos > 1) Vmem_free(thee->vmem, npos, sizeof(double), (void **)&q);
00296
00297     scale = Vunit_ec/(4*Vunit_pi*Vunit_eps0*1.0e-10);
00298     for (ipos=0; ipos<npos; ipos++) val[ipos] = val[ipos]*scale;
00299
00300     return 1;
00301
00302 #else /* ifdef HAVE_TREE */
00303
00304     return Vgreen_coulomb_direct(thee, npos, x, y, z, val);
00305 #endif
00306 }
00307
00308 }
00309
00310 VPUBLIC int Vgreen_coulombD_direct(Vgreen *thee, int npos,
00311     double *x, double *y, double *z, double *pot, double *gradx,
00312     double *grady, double *gradz) {
00313
00314     Vatom *atom;
00315     double *apos, charge, dist, dist2, idist3, dy, dz, dx, scale;
00316     double *q, qtemp;
00317     int iatom, ipos;
00318
00319     if (thee == VNULL) {
00320         Vnm_print(2, "Vgreen_coulombD: Got VNULL thee!\n");
00321         return 0;
00322     }
00323
00324     for (ipos=0; ipos<npos; ipos++) {

```

```

00325     pot[ipos] = 0.0;
00326     gradx[ipos] = 0.0;
00327     grady[ipos] = 0.0;
00328     gradz[ipos] = 0.0;
00329 }
00330
00331 for (iatom=0; iatom<Valist_getNumberAtoms(thee->alist); iatom++) {
00332     atom = Valist_getAtom(thee->alist, iatom);
00333     apos = Vatom_getPosition(atom);
00334     charge = Vatom_getCharge(atom);
00335     for (ipos=0; ipos<npos; ipos++) {
00336         dx = apos[0] - x[ipos];
00337         dy = apos[1] - y[ipos];
00338         dz = apos[2] - z[ipos];
00339         dist2 = VSQR(dx) + VSQR(dy) + VSQR(dz);
00340         dist = VSQRT(dist2);
00341         if (dist > VSMALL) {
00342             idist3 = 1.0/(dist*dist2);
00343             gradx[ipos] -= (charge*dx*idist3);
00344             grady[ipos] -= (charge*dy*idist3);
00345             gradz[ipos] -= (charge*dz*idist3);
00346             pot[ipos] += (charge/dist);
00347         }
00348     }
00349 }
00350
00351 scale = Vunit_ec/(4*VPI*Vunit_eps0*(1.0e-10));
00352 for (ipos=0; ipos<npos; ipos++) {
00353     gradx[ipos] = gradx[ipos]*scale;
00354     grady[ipos] = grady[ipos]*scale;
00355     gradz[ipos] = gradz[ipos]*scale;
00356     pot[ipos] = pot[ipos]*scale;
00357 }
00358
00359 return 1;
00360 }
00361
00362 VPUBLIC int Vgreen_coulombD(Vgreen *thee, int npos, double *x, double *y,
00363     double *z, double *pot, double *gradx, double *grady, double *gradz) {
00364
00365     Vatom *atom;
00366     double *apos, charge, dist, dist2, idist3, dy, dz, dx, scale;
00367     double *q, qtemp;
00368     int iatom, ipos;
00369
00370     if (thee == VNULL) {
00371         Vnm_print(2, "Vgreen_coulombD: Got VNULL thee!\n");
00372         return 0;
00373     }
00374
00375     for (ipos=0; ipos<npos; ipos++) {
00376         pot[ipos] = 0.0;
00377         gradx[ipos] = 0.0;
00378         grady[ipos] = 0.0;
00379         gradz[ipos] = 0.0;
00380     }
00381
00382 #ifdef HAVE_TREE
00383
00384     if (Valist_getNumberAtoms(thee->alist) > 1) {
00385         if (npos > 1) {
00386             q = VNULL;
00387             q = Vmem_malloc(thee->vmem, npos, sizeof(double));
00388             if (q == VNULL) {
00389                 Vnm_print(2, "Vgreen_coulomb: Error allocating charge array!\n");
00390                 return 0;
00391             }
00392         } else {
00393             q = &qtemp;
00394         }
00395         for (ipos=0; ipos<npos; ipos++) q[ipos] = 1.0;
00396
00397         /* Calculate */
00398         treecalc(thee, x, y, z, q, npos, pot, thee->xp, thee->yp, thee->zp,
00399             thee->qp, thee->np, gradx, grady, gradz, 2, npos, thee->np);
00400
00401         /* De-allocate charge array (if necessary) */
00402         if (npos > 1) Vmem_free(thee->vmem, npos, sizeof(double), (void **)&q);
00403     } else return Vgreen_coulombD_direct(thee, npos, x, y, z, pot,
00404         gradx, grady, gradz);
00405

```



```

00406     scale = Vunit_ec/(4*VPI*Vunit_eps0*(1.0e-10));
00407     for (ipos=0; ipos<npos; ipos++) {
00408         gradx[ipos] = gradx[ipos]*scale;
00409         grady[ipos] = grady[ipos]*scale;
00410         gradz[ipos] = gradz[ipos]*scale;
00411         pot[ipos] = pot[ipos]*scale;
00412     }
00413
00414     return 1;
00415
00416 #else /* ifdef HAVE_TREE */
00417
00418     return Vgreen_coulombD_direct(thee, npos, x, y, z, pot,
00419         gradx, grady, gradz);
00420
00421 #endif
00422 }
00423
00424
00425 VPRIVATE int treesetup(Vgreen *thee) {
00426
00427 #ifdef HAVE_TREE
00428
00429     double dist_tol = FMM_DIST_TOL;
00430     int iflag = FMM_IFLAG;
00431     double order = FMM_ORDER;
00432     int theta = FMM_THETA;
00433     int shrink = FMM_SHRINK;
00434     int maxparnode = FMM_MAXPARNODE;
00435     int minlevel = FMM_MINLEVEL;
00436     int maxlevel = FMM_MAXLEVEL;
00437     int level = 0;
00438     int one = 1;
00439     Vatom *atom;
00440     double xyzminmax[6], *pos;
00441     int i;
00442
00443     /* Set up particle arrays with atomic coordinates and charges */
00444     Vnm_print(0, "treesetup: Initializing FMM particle arrays...\n");
00445     thee->np = Valist_getNumberAtoms(thee->alist);
00446     thee->xp = VNULL;
00447     thee->xp = (double *)Vmem_malloc(thee->vmem, thee->np, sizeof(double));
00448     if (thee->xp == VNULL) {
00449         Vnm_print(2, "Vgreen_ctor2: Failed to allocate %d*sizeof(double)!\n",
00450             thee->np);
00451         return 0;
00452     }
00453     thee->yp = VNULL;
00454     thee->yp = (double *)Vmem_malloc(thee->vmem, thee->np, sizeof(double));
00455     if (thee->yp == VNULL) {
00456         Vnm_print(2, "Vgreen_ctor2: Failed to allocate %d*sizeof(double)!\n",
00457             thee->np);
00458         return 0;
00459     }
00460     thee->zp = VNULL;
00461     thee->zp = (double *)Vmem_malloc(thee->vmem, thee->np, sizeof(double));
00462     if (thee->zp == VNULL) {
00463         Vnm_print(2, "Vgreen_ctor2: Failed to allocate %d*sizeof(double)!\n",
00464             thee->np);
00465         return 0;
00466     }
00467     thee->qp = VNULL;
00468     thee->qp = (double *)Vmem_malloc(thee->vmem, thee->np, sizeof(double));
00469     if (thee->qp == VNULL) {
00470         Vnm_print(2, "Vgreen_ctor2: Failed to allocate %d*sizeof(double)!\n",
00471             thee->np);
00472         return 0;
00473     }
00474     for (i=0; i<thee->np; i++) {
00475         atom = Valist_getAtom(thee->alist, i);
00476         pos = Vatom_getPosition(atom);
00477         thee->xp[i] = pos[0];
00478         thee->yp[i] = pos[1];
00479         thee->zp[i] = pos[2];
00480         thee->qp[i] = Vatom_getCharge(atom);
00481     }
00482
00483     Vnm_print(0, "treesetup: Setting things up...\n");
00484     F77SETUP(thee->xp, thee->yp, thee->zp, &(thee->np), &order, &theta, &iflag,
00485         &dist_tol, xyzminmax, &(thee->np));
00486

```

```

00487
00488     Vnm_print(0, "treesetup: Initializing levels...\n");
00489     F77INITLEVELS(&minlevel, &maxlevel);
00490
00491     Vnm_print(0, "treesetup: Creating tree...\n");
00492     F77CREATE_TREE(&one, &(thee->np), thee->xp, thee->yp, thee->qp,
00493         &shrink, &maxparnode, xyzminmax, &level, &(thee->np));
00494
00495     return 1;
00496
00497 #else /* ifdef HAVE_TREE */
00498
00499     Vnm_print(2, "treesetup: Error! APBS not linked with treecode!\n");
00500     return 0;
00501
00502 #endif /* ifdef HAVE_TREE */
00503 }
00504
00505 VPRIVATE int treecleanup(Vgreen *thee) {
00506
00507 #ifdef HAVE_TREE
00508
00509     Vmem_free(thee->vmem, thee->np, sizeof(double), (void **)&(thee->xp));
00510     Vmem_free(thee->vmem, thee->np, sizeof(double), (void **)&(thee->yp));
00511     Vmem_free(thee->vmem, thee->np, sizeof(double), (void **)&(thee->zp));
00512     Vmem_free(thee->vmem, thee->np, sizeof(double), (void **)&(thee->qp));
00513     F77CLEANUP();
00514
00515     return 1;
00516
00517 #else /* ifdef HAVE_TREE */
00518
00519     Vnm_print(2, "treecleanup: Error! APBS not linked with treecode!\n");
00520     return 0;
00521
00522 #endif /* ifdef HAVE_TREE */
00523 }
00524
00525 VPRIVATE int treecalc(Vgreen *thee, double *xtar, double *ytar, double *ztar,
00526     double *qtar, int numtars, double *tpengtar, double *x, double *y,
00527     double *z, double *q, int numpars, double *fx, double *fy, double *fz,
00528     int iflag, int farrdim, int arrdim) {
00529
00530 #ifdef HAVE_TREE
00531     int i, level, err, maxlevel, minlevel, one;
00532     double xyzminmax[6];
00533
00534
00535     if (iflag != 1) {
00536         F77TREE_COMPP(xtar, ytar, ztar, qtar, &numtars, tpengtar, x, y, z, q,
00537             fx, fy, fz, &numpars, &farrdim, &arrdim);
00538     } else {
00539         F77TREE_COMPP(xtar, ytar, ztar, qtar, &numtars, tpengtar, &farrdim, x,
00540             y, z, q, &numpars, &arrdim);
00541     }
00542
00543
00544     return 1;
00545
00546 #else /* ifdef HAVE_TREE */
00547
00548     Vnm_print(2, "treecalc: Error! APBS not linked with treecode!\n");
00549     return 0;
00550
00551 #endif /* ifdef HAVE_TREE */
00552 }

```

9.72 src/generic/vgreen.h File Reference

Contains declarations for class Vgreen.

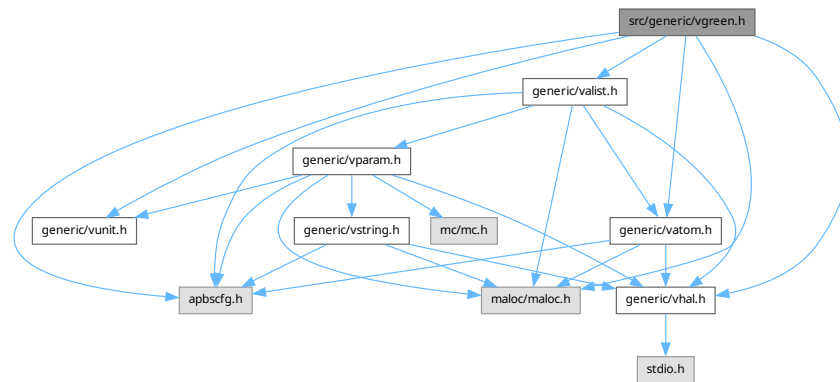
```

#include "apbscfg.h"
#include "malloc/malloc.h"
#include "generic/vhal.h"
#include "generic/vunit.h"
#include "generic/vatom.h"

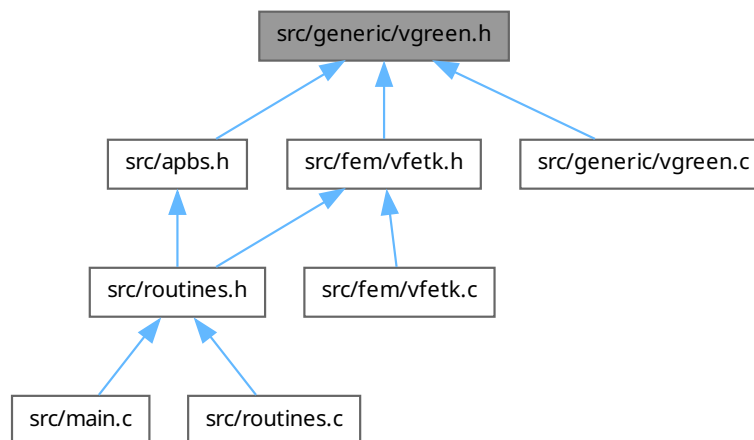
```

```
#include "generic/valist.h"
```

Include dependency graph for vgreen.h:



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [sVgreen](#)
Contains public data members for Vgreen class/module.

Typedefs

- typedef struct [sVgreen](#) [Vgreen](#)
Declaration of the Vgreen class as the Vgreen structure.

Functions

- VEXTERNC Valist * Vgreen_getValist (Vgreen *thee)

Get the atom list associated with this Green's function object.
- VEXTERNC unsigned long int Vgreen_memChk (Vgreen *thee)

Return the memory used by this structure (and its contents) in bytes.
- VEXTERNC Vgreen * Vgreen_ctor (Valist *alist)

Construct the Green's function oracle.
- VEXTERNC int Vgreen_ctor2 (Vgreen *thee, Valist *alist)

FORTTRAN stub to construct the Green's function oracle.
- VEXTERNC void Vgreen_dtor (Vgreen **thee)

Destruct the Green's function oracle.
- VEXTERNC void Vgreen_dtor2 (Vgreen *thee)

FORTTRAN stub to destruct the Green's function oracle.
- VEXTERNC int Vgreen_helmholtz (Vgreen *thee, int npos, double *x, double *y, double *z, double *val, double kappa)

Get the Green's function for Helmholtz's equation integrated over the atomic point charges.
- VEXTERNC int Vgreen_helmholtzD (Vgreen *thee, int npos, double *x, double *y, double *z, double *gradx, double *grady, double *gradz, double kappa)

Get the gradient of Green's function for Helmholtz's equation integrated over the atomic point charges.
- VEXTERNC int Vgreen_coulomb_direct (Vgreen *thee, int npos, double *x, double *y, double *z, double *val)

Get the Coulomb's Law Green's function (solution to Laplace's equation) integrated over the atomic point charges using direct summation.
- VEXTERNC int Vgreen_coulomb (Vgreen *thee, int npos, double *x, double *y, double *z, double *val)

Get the Coulomb's Law Green's function (solution to Laplace's equation) integrated over the atomic point charges using direct summation or H. E. Johnston, R. Krasny FMM library (if available)
- VEXTERNC int Vgreen_coulombD_direct (Vgreen *thee, int npos, double *x, double *y, double *z, double *pot, double *gradx, double *grady, double *gradz)

Get gradient of the Coulomb's Law Green's function (solution to Laplace's equation) integrated over the atomic point charges using direct summation.
- VEXTERNC int Vgreen_coulombD (Vgreen *thee, int npos, double *x, double *y, double *z, double *pot, double *gradx, double *grady, double *gradz)

Get gradient of the Coulomb's Law Green's function (solution to Laplace's equation) integrated over the atomic point charges using either direct summation or H. E. Johnston/R. Krasny FMM library (if available)

9.72.1 Detailed Description

Contains declarations for class Vgreen.

Version

\$Id\$

Author

Nathan A. Baker

Definition in file [vgreen.h](#).

9.73 vgreen.h

[Go to the documentation of this file.](#)

```

00001
00065 #ifndef _VGREEN_H_
00066 #define _VGREEN_H_
00067
00068 #include "apbscfg.h"
00069
00070 #include "malloc/malloc.h"
00071
00072 #include "generic/vhal.h"
00073 #include "generic/vunit.h"
00074 #include "generic/vatom.h"
00075 #include "generic/valist.h"
00076
00082 struct sVgreen {
00083
00084     Valist *alist;
00085     Vmem *vmem;
00086     double *xp;
00088     double *yp;
00090     double *zp;
00092     double *qp;
00094     int np;
00095 };
00096
00101 typedef struct sVgreen Vgreen;
00102
00103 /* ////////////////////////////////////////
00104 // Class Vgreen: Inlineable methods (vgreen.c)
00106
00107 #if !defined(VINLINE_VGREEN)
00108
00116     VEXTERNC Valist* Vgreen_getValist(Vgreen *thee);
00117
00125     VEXTERNC unsigned long int Vgreen_memChk(Vgreen *thee);
00126
00127 #else /* if defined(VINLINE_VGREEN) */
00128 #   define Vgreen_getValist(thee) ((thee)->alist)
00129 #   define Vgreen_memChk(thee) (Vmem_bytes((thee)->vmem))
00130 #endif /* if !defined(VINLINE_VGREEN) */
00131
00132 /* ////////////////////////////////////////
00133 // Class Vgreen: Non-Inlineable methods (vgreen.c)
00135
00142 VEXTERNC Vgreen* Vgreen_ctor(Valist *alist);
00143
00151 VEXTERNC int Vgreen_ctor2(Vgreen *thee, Valist *alist);
00152
00158 VEXTERNC void Vgreen_dtor(Vgreen **thee);
00159
00165 VEXTERNC void Vgreen_dtor2(Vgreen *thee);
00166
00191 VEXTERNC int Vgreen_helmholtz(Vgreen *thee, int npos, double *x, double *y,
00192     double *z, double *val, double kappa);
00193
00221 VEXTERNC int Vgreen_helmholtzD(Vgreen *thee, int npos, double *x, double *y,
00222     double *z, double *gradx, double *grady, double *gradz, double kappa);
00223
00244 VEXTERNC int Vgreen_coulomb_direct(Vgreen *thee, int npos, double *x,
00245     double *y, double *z, double *val);
00246
00267 VEXTERNC int Vgreen_coulomb(Vgreen *thee, int npos, double *x, double *y,
00268     double *z, double *val);
00269
00293 VEXTERNC int Vgreen_coulombD_direct(Vgreen *thee, int npos, double *x,
00294     double *y, double *z, double *pot, double *gradx, double *grady, double
00295     *gradz);
00296
00321 VEXTERNC int Vgreen_coulombD(Vgreen *thee, int npos, double *x, double *y,
00322     double *z, double *pot, double *gradx, double *grady, double *gradz);
00323
00324 #endif /* ifndef _VGREEN_H_ */

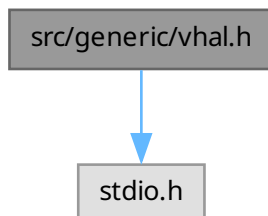
```

9.74 src/generic/vhal.h File Reference

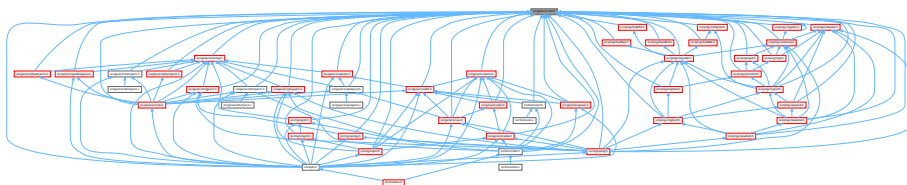
Contains generic macro definitions for APBS.

```
#include "stdio.h"
```

Include dependency graph for vhal.h:



This graph shows which files directly or indirectly include this file:



Macros

- `#define APBS_TIMER_WALL_CLOCK` 26
APBS total execution timer ID.
- `#define APBS_TIMER_SETUP` 27
APBS setup timer ID.
- `#define APBS_TIMER_SOLVER` 28
APBS solver timer ID.
- `#define APBS_TIMER_ENERGY` 29
APBS energy timer ID.
- `#define APBS_TIMER_FORCE` 30
APBS force timer ID.
- `#define APBS_TIMER_TEMP1` 31
APBS temp timer #1 ID.
- `#define APBS_TIMER_TEMP2` 32
APBS temp timer #2 ID.
- `#define MAXMOL` 5
The maximum number of molecules that can be involved in a single PBE calculation.
- `#define MAXION` 10
The maximum number of ion species that can be involved in a single PBE calculation.

- #define `MAXFOCUS` 5
The maximum number of times an MG calculation can be focused.
- #define `VMGNLEV` 4
Minimum number of levels in a multigrid calculations.
- #define `VREDFRAC` 0.25
Maximum reduction of grid spacing during a focusing calculation.
- #define `VAPBS_NVS` 4
Number of vertices per simplex (hard-coded to 3D)
- #define `VAPBS_DIM` 3
Our dimension.
- #define `VAPBS_RIGHT` 0
Face definition for a volume.
- #define `VAPBS_FRONT` 1
Face definition for a volume.
- #define `VAPBS_UP` 2
Face definition for a volume.
- #define `VAPBS_LEFT` 3
Face definition for a volume.
- #define `VAPBS_BACK` 4
Face definition for a volume.
- #define `VAPBS_DOWN` 5
Face definition for a volume.
- #define `VPMGSMALL` 1e-12
A small number used in Vpmg to decide if points are on/off grid-lines or non-zero (etc.)
- #define `SINH_MIN` -85.0
Used to set the min values acceptable for sinh chopping.
- #define `SINH_MAX` 85.0
Used to set the max values acceptable for sinh chopping.
- #define `MAX_HASH_DIM` 75
- #define `VF77_MANGLE`(name, NAME) name
Name-mangling macro for using FORTRAN functions in C code.
- #define `VFLOOR`(value) floor(value)
Wrapped floor to fix floating point issues in the Intel compiler.
- #define `VEMBED`(rctag)
Allows embedding of RCS ID tags in object files.
- #define `PRINT_FUNC` __PRETTY_FUNCTION__
- #define `OS_SEP_STR` "/"
- #define `OS_SEP_CHAR` '/'
- #define `ANNOUNCE_FUNCTION`
- #define `WARN_UNTESTED`
- #define `WARN_PARTTESTED`
- #define `VCHANNELEDMESSAGE0`(channel, msg)
- #define `VCHANNELEDMESSAGE1`(channel, msg, arg0)
- #define `VCHANNELEDMESSAGE2`(channel, msg, arg0, arg1)
- #define `VCHANNELEDMESSAGE3`(channel, msg, arg0, arg1, arg2)
- #define `VMESSAGE0`(msg) VCHANNELEDMESSAGE0(0, msg)
- #define `VMESSAGE1`(msg, arg0) VCHANNELEDMESSAGE1(0, msg, arg0)
- #define `VMESSAGE2`(msg, arg0, arg1) VCHANNELEDMESSAGE2(0, msg, arg0, arg1)

- #define [VMESSAGE3](#)(msg, arg0, arg1, arg2) VCHANNELEDMESSAGE3(0, msg, arg0, arg1, arg2)
- #define [VERRMSG0](#)(msg) VCHANNELEDMESSAGE0(2, msg)
- #define [VERRMSG1](#)(msg, arg0) VCHANNELEDMESSAGE1(2, msg, arg0)
- #define [VERRMSG2](#)(msg, arg0, arg1) VCHANNELEDMESSAGE2(2, msg, arg0, arg1)
- #define [VERRMSG3](#)(msg, arg0, arg1, arg2) VCHANNELEDMESSAGE3(2, msg, arg0, arg1, arg2)
- #define [VASSERT_MSG0](#)(cnd, msg)
- #define [VASSERT_MSG1](#)(cnd, msg, arg)
- #define [VASSERT_MSG2](#)(cnd, msg, arg0, arg1)
- #define [VWARN_MSG0](#)(cnd, msg)
- #define [VWARN_MSG1](#)(cnd, msg, arg0)
- #define [VWARN_MSG2](#)(cnd, msg, arg0, arg1)
- #define [VABORT_MSG0](#)(msg)
- #define [VABORT_MSG1](#)(msg, arg)
- #define [VABORT_MSG2](#)(msg, arg0, arg1)
- #define [PRINT_INT](#)(expr)
- #define [PRINT_DBL](#)(expr)
- #define [VMALLOC](#)(vmem, n, type) ((type*)Vmem_malloc(vmem, n, sizeof(type)))
- #define [VFREE](#)(vmem, n, type, ptr) (Vmem_free(vmem, n, sizeof(type), (void **)&(ptr)))
- #define [VFILL](#)(vec, n, val)
- #define [VCOPY](#)(srcvec, dstvec, i, n)
- #define [VAT](#)(array, i) ((array)[i] - 1)
- #define [RAT](#)(array, i) ((array) + i - 1)

Typedefs

- typedef enum [eVrc_Codes](#) [Vrc_Codes](#)
- typedef enum [eVsol_Meth](#) [Vsol_Meth](#)
- typedef enum [eVsurf_Meth](#) [Vsurf_Meth](#)
- typedef enum [eVhal_PBEType](#) [Vhal_PBEType](#)
Declaration of the Vhal_PBEType type as the Vhal_PBEType enum.
- typedef enum [eVhal_IPKEYType](#) [Vhal_IPKEYType](#)
Declaration of the Vhal_IPKEYType type as the Vhal_IPKEYType enum.
- typedef enum [eVhal_NONLINType](#) [Vhal_NONLINType](#)
Declaration of the Vhal_NONLINType type as the Vhal_NONLINType enum.
- typedef enum [eVoutput_Format](#) [Voutput_Format](#)
Declaration of the Voutput_Format type as the VOutput_Format enum.
- typedef enum [eVbcfl](#) [Vbcfl](#)
Declare Vbcfl type.
- typedef enum [eVchrg_Meth](#) [Vchrg_Meth](#)
- typedef enum [eVchrg_Src](#) [Vchrg_Src](#)
- typedef enum [eVdata_Type](#) [Vdata_Type](#)
- typedef enum [eVdata_Format](#) [Vdata_Format](#)

Enumerations

- enum `eVrc_Codes` { `VRC_WARNING` = -1 , `VRC_FAILURE` = 0 , `VRC_SUCCESS` = 1 }
Return code enumerations.
- enum `eVsol_Meth` {
 `VSOL_CGMG` , `VSOL_Newton` , `VSOL_MG` , `VSOL_CG` ,
 `VSOL_SOR` , `VSOL_RBGS` , `VSOL_WJ` , `VSOL_Richardson` ,
 `VSOL_CGMGAqua` , `VSOL_NewtonAqua` }
Solution Method enumerations.
- enum `eVsurf_Meth` {
 `VSM_MOL` = 0 , `VSM_MOLSMOOTH` = 1 , `VSM_SPLINE` = 2 , `VSM_SPLINE3` = 3 ,
 `VSM_SPLINE4` = 4 }
Types of molecular surface definitions.
- enum `eVhal_PBEType` {
 `PBE_LPBE` , `PBE_NPBE` , `PBE_LRPBE` , `PBE_NRPBE` ,
 `PBE_SMPBE` }
Version of PBE to solve.
- enum `eVhal_IPKEYType` { `IPKEY_SMPBE` = -2 , `IPKEY_LPBE` , `IPKEY_NPBE` }
Type of ipkey to use for MG methods.
- enum `eVhal_NONLINType` {
 `NONLIN_LPBE` = 0 , `NONLIN_NPBE` , `NONLIN_SMPBE` , `NONLIN_LPBEAQUA` ,
 `NONLIN_NPBEAQUA` }
Type of nonlinear to use for MG methods.
- enum `eVoutput_Format` { `OUTPUT_NULL` , `OUTPUT_FLAT` }
Output file format.
- enum `eVbcfl` {
 `BCFL_ZERO` = 0 , `BCFL_SDH` = 1 , `BCFL_MDH` = 2 , `BCFL_UNUSED` = 3 ,
 `BCFL_FOCUS` = 4 , `BCFL_MEM` = 5 , `BCFL_MAP` = 6 }
Types of boundary conditions.
- enum `eVchrg_Meth` { `VCM_TRIL` = 0 , `VCM_BSPL2` = 1 , `VCM_BSPL4` = 2 }
Types of charge discretization methods.
- enum `eVchrg_Src` { `VCM_CHARGE` = 0 , `VCM_PERMANENT` = 1 , `VCM_INDUCED` = 2 , `VCM_NLINDUCED` = 3 }
Charge source.
- enum `eVdata_Type` {
 `VDT_CHARGE` , `VDT_POT` , `VDT_ATOMPOT` , `VDT_SMOL` ,
 `VDT_SSPL` , `VDT_VDW` , `VDT_IVDW` , `VDT_LAP` ,
 `VDT_EDENS` , `VDT_NDENS` , `VDT_QDENS` , `VDT_DIELX` ,
 `VDT_DIELY` , `VDT_DIELZ` , `VDT_KAPPA` }
Types of (scalar) data that can be written out of APBS.
- enum `eVdata_Format` {
 `VDF_DX` = 0 , `VDF_UHBD` = 1 , `VDF_AVS` = 2 , `VDF_MCSF` = 3 ,
 `VDF_GZ` = 4 , `VDF_FLAT` = 5 , `VDF_DXBIN` = 6 }
Format of data for APBS I/O.

Functions

- `char * wrap_text` (char *str, int right_margin, int left_padding)

9.74.1 Detailed Description

Contains generic macro definitions for APBS.

Version

\$Id\$

Author

Nathan A. Baker

Attention

```
*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
* Nathan A. Baker (nathan.baker@pnl.gov)
* Pacific Northwest National Laboratory
*
* Additional contributing authors listed in the code documentation.
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*
*
```

Definition in file [vhal.h](#).

9.74.2 Macro Definition Documentation

9.74.2.1 ANNOUNCE_FUNCTION

```
#define ANNOUNCE_FUNCTION
```

Definition at line 600 of file [vhal.h](#).

9.74.2.2 MAX_HASH_DIM

```
#define MAX_HASH_DIM 75
```

Definition at line 458 of file [vhal.h](#).

9.74.2.3 OS_SEP_CHAR

```
#define OS_SEP_CHAR '/'
```

Definition at line 573 of file [vhal.h](#).

9.74.2.4 OS_SEP_STR

```
#define OS_SEP_STR "/"
```

Definition at line 572 of file [vhal.h](#).

9.74.2.5 PRINT_DBL

```
#define PRINT_DBL(  
    expr )
```

Definition at line 945 of file [vhal.h](#).

9.74.2.6 PRINT_FUNC

```
#define PRINT_FUNC __PRETTY_FUNCTION__
```

OS specific flags and etcetera

Definition at line 571 of file [vhal.h](#).

9.74.2.7 PRINT_INT

```
#define PRINT_INT(  
    expr )
```

Definition at line 944 of file [vhal.h](#).

9.74.2.8 RAT

```
#define RAT(  
    array,  
    i ) ((array) + i - 1)
```

Definition at line 969 of file [vhal.h](#).

9.74.2.9 VABORT_MSG0

```
#define VABORT_MSG0(  
    msg )
```

Value:

```
do {  
    Vnm_print(2, "[%s()]: ABORTING:\n" \  
              "%s\n\n", \  
              __FUNCTION__, msg); \  
    abort();  
} while(0)
```

Definition at line 899 of file [vhal.h](#).

9.74.2.10 VABORT_MSG1

```
#define VABORT_MSG1(  
    msg,  
    arg )
```

Value:

```
do {  
    char buff[1000];  
    snprintf( buff, 1000, msg, arg );  
    Vnm_print(2, "[%s()]: ABORTING:\n" \  
              "%s\n\n", \  
              __FUNCTION__, buff); \
```

```
        abort();
    } while(0) \
```

Definition at line 907 of file [vhal.h](#).

9.74.2.11 VABORT_MSG2

```
#define VABORT_MSG2(  
    msg,  
    arg0,  
    arg1 )
```

Value:

```
do {  
    char buff[1000];  
    snprintf( buff, 1000, msg, arg0, arg1);  
    Vnm_print(2, "[%s()]: ABORTING:\n"  
        "    %s\n\n",  
        __FUNCTION__, buff);  
    abort();  
} while(0) \
```

Definition at line 917 of file [vhal.h](#).

9.74.2.12 VASSERT_MSG0

```
#define VASSERT_MSG0(  
    cnd,  
    msg )
```

Value:

```
do {  
    if( (cnd) == 0 ) {  
        Vnm_print(2, "[%s()]: ERROR:\n"  
            "    Assertion Failed (%s): %s\n\n",  
            __FUNCTION__, #cnd, msg);  
        abort();  
    }  
} while(0) \
```

Definition at line 731 of file [vhal.h](#).

9.74.2.13 VASSERT_MSG1

```
#define VASSERT_MSG1(  
    cnd,  
    msg,  
    arg )
```

Value:

```
do {  
    if( (cnd) == 0 ) {  
        char buff[1000];  
        snprintf( buff, 1000, msg, arg );  
        Vnm_print(2, "[%s()]: ERROR:\n"  
            "    Assertion Failed (%s): %s\n\n",  
            __FUNCTION__, #cnd, buff);  
        abort();  
    }  
} while(0) \
```

Definition at line 741 of file [vhal.h](#).

9.74.2.14 VASSERT_MSG2

```
#define VASSERT_MSG2(  
    cnd,  
    msg,  
    arg0,  
    arg1 )
```

Value:

```

do {
    if( (cnd) == 0 ) {
        char buff[1000];
        snprintf( buff, 1000, msg, arg0, arg1 );
        Vnm_print(2, "[%s()]: ERROR:\n"
                  "    Assertion Failed (%s): %s\n\n",
                  __FUNCTION__, #cnd, buff);
        abort();
    }
} while(0)

```

Definition at line 753 of file [vhal.h](#).

9.74.2.15 VAT

```

#define VAT(
    array,
    i ) ((array)[(i) - 1])

```

Definition at line 968 of file [vhal.h](#).

9.74.2.16 VCHANNELEDMESSAGE0

```

#define VCHANNELEDMESSAGE0(
    channel,
    msg )

```

Value:

```

do {
    Vnm_print(channel, "%s: %s\n", __FUNCTION__, msg); \
} while(0)

```

Definition at line 653 of file [vhal.h](#).

9.74.2.17 VCHANNELEDMESSAGE1

```

#define VCHANNELEDMESSAGE1(
    channel,
    msg,
    arg0 )

```

Value:

```

do {
    char buff[1000];
    snprintf( buff, 1000, msg, arg0 );
    Vnm_print(channel, "%s: %s\n", __FUNCTION__, buff); \
} while(0)

```

Definition at line 658 of file [vhal.h](#).

9.74.2.18 VCHANNELEDMESSAGE2

```

#define VCHANNELEDMESSAGE2(
    channel,
    msg,
    arg0,
    arg1 )

```

Value:

```

do {
    char buff[1000];
    snprintf( buff, 1000, msg, arg0, arg1 );
    Vnm_print(channel, "%s: %s\n", __FUNCTION__, buff); \
} while(0)

```

Definition at line 665 of file [vhal.h](#).

9.74.2.19 VCHANNELEDMESSAGE3

```

#define VCHANNELEDMESSAGE3(

```

```

channel,
msg,
arg0,
arg1,
arg2 )

```

Value:

```

do {
    char buff[1000];
    snprintf(buff, 1000, msg, arg0, arg1, arg2);
    Vnm_print(channel, "%s: %s\n", __FUNCTION__, buff);
} while(0)

```

Definition at line 672 of file [vhal.h](#).

9.74.2.20 VCOPY

```

#define VCOPY(
    srcvec,
    dstvec,
    i,
    n )

```

Value:

```

do {
    for (i = 0; i < n; i++)
        dstvec[i] = srcvec[i];
} while(0)

```

Definition at line 959 of file [vhal.h](#).

9.74.2.21 VERRMSG0

```

#define VERRMSG0(
    msg ) VCHANNELEDMESSAGE0(2, msg)

```

Definition at line 684 of file [vhal.h](#).

9.74.2.22 VERRMSG1

```

#define VERRMSG1(
    msg,
    arg0 ) VCHANNELEDMESSAGE1(2, msg, arg0)

```

Definition at line 685 of file [vhal.h](#).

9.74.2.23 VERRMSG2

```

#define VERRMSG2(
    msg,
    arg0,
    arg1 ) VCHANNELEDMESSAGE2(2, msg, arg0, arg1)

```

Definition at line 686 of file [vhal.h](#).

9.74.2.24 VERRMSG3

```

#define VERRMSG3(
    msg,
    arg0,
    arg1,
    arg2 ) VCHANNELEDMESSAGE3(2, msg, arg0, arg1, arg2)

```

Definition at line 687 of file [vhal.h](#).

9.74.2.25 VFILL

```
#define VFILL(
    vec,
    n,
    val )
```

Value:

```
do {
    int fill_idx;
    for (fill_idx = 0; fill_idx < n; fill_idx++) \
        vec[fill_idx] = val;
} while(0)
```

Definition at line 952 of file [vhal.h](#).

9.74.2.26 VFREE

```
#define VFREE(
    vmem,
    n,
    type,
    ptr ) (Vmem_free(vmem, n, sizeof(type), (void **)&(ptr)))
```

Definition at line 950 of file [vhal.h](#).

9.74.2.27 VMALLOC

```
#define VMALLOC(
    vmem,
    n,
    type ) ((type*)Vmem_malloc(vmem, n, sizeof(type)))
```

Definition at line 948 of file [vhal.h](#).

9.74.2.28 VMESSAGE0

```
#define VMESSAGE0(
    msg ) VCHANNELEDMESSAGE0(0, msg)
```

Definition at line 679 of file [vhal.h](#).

9.74.2.29 VMESSAGE1

```
#define VMESSAGE1(
    msg,
    arg0 ) VCHANNELEDMESSAGE1(0, msg, arg0)
```

Definition at line 680 of file [vhal.h](#).

9.74.2.30 VMESSAGE2

```
#define VMESSAGE2(
    msg,
    arg0,
    arg1 ) VCHANNELEDMESSAGE2(0, msg, arg0, arg1)
```

Definition at line 681 of file [vhal.h](#).

9.74.2.31 VMESSAGE3

```
#define VMESSAGE3(
    msg,
    arg0,
```

```

    arg1,
    arg2 ) VCHANNELEDMESSAGE3(0, msg, arg0, arg1, arg2)

```

Definition at line 682 of file [vhal.h](#).

9.74.2.32 VWARN_MSG0

```

#define VWARN_MSG0(
    cnd,
    msg )

```

Value:

```

do {
    if( (cnd) == 0 ) {
        Vnm_print(
            2,
            "[%s()]: WARNING:\n"
            "    %s\n\n",
            __FUNCTION__,
            msg
        );
    }
} while(0)

```

Definition at line 825 of file [vhal.h](#).

9.74.2.33 VWARN_MSG1

```

#define VWARN_MSG1(
    cnd,
    msg,
    arg0 )

```

Value:

```

do {
    if( (cnd) == 0 ) {
        char buff[1000];
        snprintf(buff, 1000, msg, arg0);
        Vnm_print(
            2,
            "[%s()]: WARNING:\n"
            "    %s\n\n",
            __FUNCTION__,
            buff
        );
    }
} while(0)

```

Definition at line 838 of file [vhal.h](#).

9.74.2.34 VWARN_MSG2

```

#define VWARN_MSG2(
    cnd,
    msg,
    arg0,
    arg1 )

```

Value:

```

do {
    if( (cnd) == 0 ) {
        char buff[1000];
        snprintf(buff, 1000, msg, arg0, arg1);
        Vnm_print(
            2,
            "[%s()]: WARNING:\n"
            "    %s\n\n",
            __FUNCTION__,
            buff
        );
    }
} while(0)

```

Definition at line 853 of file [vhal.h](#).

9.74.2.35 WARN_PARTTESTED

```
#define WARN_PARTTESTED
```

Definition at line 602 of file [vhal.h](#).

9.74.2.36 WARN_UNTESTED

```
#define WARN_UNTESTED
```

Definition at line 601 of file [vhal.h](#).

9.74.3 Typedef Documentation

9.74.3.1 Vchrg_Meth

```
typedef enum eVchrg_Meth Vchrg_Meth
```

Definition at line 244 of file [vhal.h](#).

9.74.3.2 Vchrg_Src

```
typedef enum eVchrg_Src Vchrg_Src
```

Definition at line 262 of file [vhal.h](#).

9.74.3.3 Vdata_Format

```
typedef enum eVdata_Format Vdata_Format
```

Definition at line 323 of file [vhal.h](#).

9.74.3.4 Vdata_Type

```
typedef enum eVdata_Type Vdata_Type
```

Definition at line 302 of file [vhal.h](#).

9.74.3.5 Vrc_Codes

```
typedef enum eVrc_Codes Vrc_Codes
```

Definition at line 73 of file [vhal.h](#).

9.74.3.6 Vsol_Meth

```
typedef enum eVsol_Meth Vsol_Meth
```

Definition at line 95 of file [vhal.h](#).

9.74.3.7 Vsurf_Meth

```
typedef enum eVsurf_Meth Vsurf_Meth
```

Definition at line 133 of file [vhal.h](#).

9.75 vhal.h

[Go to the documentation of this file.](#)

```
00001
00055 #ifndef _VAPBSHAL_H_
00056 #define _VAPBSHAL_H_
00057
00058 #include "stdio.h"
00059
00066 enum eVrc_Codes {
00067
```

```

00068     VRC_WARNING=-1,
00069     VRC_FAILURE=0,
00070     VRC_SUCCESS=1
00072 };
00073 typedef enum eVrc_Codes Vrc_Codes;
00074
00081 enum eVsol_Meth {
00082
00083     VSOL_CGMG,          /* 0: conjugate gradient multigrid */
00084     VSOL_Newton,        /* 1: newton */
00085     VSOL_MG,            /* 2: multigrid */
00086     VSOL_CG,            /* 3: conjugate gradient */
00087     VSOL_SOR,           /* 4: successive overrelaxation */
00088     VSOL_RBGS,          /* 5: red-black gauss-seidel */
00089     VSOL_WJ,            /* 6: weighted jacobi */
00090     VSOL_Richardson,    /* 7: richardson */
00091     VSOL_CGMGAqua,      /* 8: conjugate gradient multigrid aqua */
00092     VSOL_NewtonAqua     /* 9: newton aqua */
00093
00094 };
00095 typedef enum eVsol_Meth Vsol_Meth;
00096
00102 enum eVsurf_Meth {
00103     VSM_MOL=0,
00107     VSM_MOLSMOOTH=1,
00109     VSM_SPLINE=2,
00119     VSM_SPLINE3=3,
00123     VSM_SPLINE4=4
00127 };
00128
00133 typedef enum eVsurf_Meth Vsurf_Meth;
00134
00139 enum eVhal_PBEType {
00140     PBE_LPBE,
00141     PBE_NPBE,
00142     PBE_LRPBE,
00143     PBE_NRPBE,
00144     PBE_SMPBE
00145 };
00146
00151 typedef enum eVhal_PBEType Vhal_PBEType;
00152
00157 enum eVhal_IPKEYType {
00158     IPKEY_SMPBE = -2,
00159     IPKEY_LPBE,
00160     IPKEY_NPBE
00161 };
00162
00167 typedef enum eVhal_IPKEYType Vhal_IPKEYType;
00168
00173 enum eVhal_NONLINType {
00174     NONLIN_LPBE = 0,
00175     NONLIN_NPBE,
00176     NONLIN_SMPBE,
00177     NONLIN_LPBEAQUA,
00178     NONLIN_NPBEAQUA
00179 };
00180
00185 typedef enum eVhal_NONLINType Vhal_NONLINType;
00186
00191 enum eVoutput_Format {
00192     OUTPUT_NULL,
00193     OUTPUT_FLAT,
00194 };
00195
00200 typedef enum eVoutput_Format Voutput_Format;
00201
00207 enum eVbcfl {
00208     BCFL_ZERO=0,
00209     BCFL_SDH=1,
00211     BCFL_MDH=2,
00213     BCFL_UNUSED=3,
00214     BCFL_FOCUS=4,
00215     BCFL_MEM=5,
00216     BCFL_MAP=6
00217 };
00218
00223 typedef enum eVbcfl Vbcfl;
00224
00230 enum eVchrg_Meth {
00231     VCM_TRIL=0,

```

```
00234     VCM_BSPL2=1,
00237     VCM_BSPL4=2
00238 };
00239
00244 typedef enum eVchrg_Meth Vchrg_Meth;
00245
00251 enum eVchrg_Src {
00252     VCM_CHARGE=0,
00253     VCM_PERMANENT=1,
00254     VCM_INDUCED=2,
00255     VCM_NLINDUCED=3
00256 };
00257
00262 typedef enum eVchrg_Src Vchrg_Src;
00263
00269 enum eVdata_Type {
00270     VDT_CHARGE,
00271     VDT_POT,
00272     VDT_ATOMPOT,
00273     VDT_SMOL,
00275     VDT_SSPL,
00277     VDT_VDW,
00279     VDT_IVDW,
00281     VDT_LAP,
00282     VDT_EDENS,
00284     VDT_NDENS,
00286     VDT_QDENS,
00288     VDT_DIELX,
00290     VDT_DIELY,
00292     VDT_DIELZ,
00294     VDT_KAPPA
00296 };
00297
00302 typedef enum eVdata_Type Vdata_Type;
00303
00309 enum eVdata_Format {
00310     VDF_DX=0,
00311     VDF_UHBD=1,
00312     VDF_AVS=2,
00313     VDF_MCSF=3,
00314     VDF_GZ=4,
00315     VDF_FLAT=5,
00316     VDF_DXBIN=6
00317 };
00318
00323 typedef enum eVdata_Format Vdata_Format;
00324
00329 #define APBS_TIMER_WALL_CLOCK 26
00330
00335 #define APBS_TIMER_SETUP 27
00336
00341 #define APBS_TIMER_SOLVER 28
00342
00347 #define APBS_TIMER_ENERGY 29
00348
00353 #define APBS_TIMER_FORCE 30
00354
00359 #define APBS_TIMER_TEMP1 31
00360
00365 #define APBS_TIMER_TEMP2 32
00366
00371 #define MAXMOL 5
00372
00377 #define MAXION 10
00378
00382 #define MAXFOCUS 5
00383
00387 #define VMGNLEV 4
00388
00392 #define VREDFRAC 0.25
00393
00397 #define VAPBS_NVS 4
00398
00402 #define VAPBS_DIM 3
00403
00408 #define VAPBS_RIGHT 0
00409
00414 #define VAPBS_FRONT 1
00415
00420 #define VAPBS_UP 2
00421
```

```

00426 #define VAPBS_LEFT 3
00427
00432 #define VAPBS_BACK 4
00433
00438 #define VAPBS_DOWN 5
00439
00444 #define VPMGSMALL 1e-12
00445
00450 #define SINH_MIN -85.0
00451
00456 #define SINH_MAX 85.0
00457
00458 #define MAX_HASH_DIM 75
00459
00460 #if defined(VDEBUG)
00461 #   if !defined(APBS_NOINLINE)
00462 #       define APBS_NOINLINE 1
00463 #   endif
00464 #endif
00465
00466 #if !defined(APBS_NOINLINE)
00467
00471 #   define VINLINE_VACC
00472
00476 #   define VINLINE_VATOM
00477
00481 #   define VINLINE_VCSM
00482
00486 #   define VINLINE_VPBE
00487
00491 #   define VINLINE_VPEE
00492
00496 #   define VINLINE_VGREEN
00497
00501 #   define VINLINE_VFETK
00502
00506 #   define VINLINE_VPMG
00507
00512 #endif
00513
00514 /* Fortran name mangling */
00515 #if defined(VF77_UPPERCASE)
00516 #   if defined(VF77_NOUNDERSCORE)
00517 #       define VF77_MANGLE(name,NAME) NAME
00518 #   elif defined(VF77_ONEUNDERSCORE)
00519 #       define VF77_MANGLE(name,NAME) NAME ## _
00520 #   else
00521 #       define VF77_MANGLE(name,NAME) name
00522 #   endif
00523 #else
00524 #   if defined(VF77_NOUNDERSCORE)
00525 #       define VF77_MANGLE(name,NAME) name
00526 #   elif defined(VF77_ONEUNDERSCORE)
00527 #       define VF77_MANGLE(name,NAME) name ## _
00528 #   else
00532 #       define VF77_MANGLE(name,NAME) name
00533 #   endif
00534 #endif
00535
00536 /* Floating Point Error */
00537 #if defined(FLOAT_EPSILON)
00538 #   define VFLOOR(value) \
00539       ((floor(value) != floor(value + FLOAT_EPSILON)) ? \
00540        floor(value + FLOAT_EPSILON) : floor(value))
00541 #else
00547 #   define VFLOOR(value) floor(value)
00548 #endif
00549
00550 /* String embedding for ident */
00551 #if defined(HAVE_EMBED)
00556 #   define VEMBED(rctag) \
00557       VPRIVATE const char* rctag; \
00558       static void* use_rcsid=(0 ? &use_rcsid : (void*)&rcsid);
00559 #else
00564 #   define VEMBED(rctag)
00565 #endif /* if defined(HAVE_EMBED) */
00566
00567
00568
00570 #if !defined(_WIN32) || defined(__MINGW32__)
00571 #define PRINT_FUNC __PRETTY_FUNCTION__

```

```

00572 #define OS_SEP_STR "/"
00573 #define OS_SEP_CHAR '/'
00574 #else
00575 #define OS_SEP_STR "\\\"
00576 #define OS_SEP_CHAR '\\\"
00577 #define PRINT_FUNC __FUNCSIG__
00578 #define snprintf sprintf_s
00579 #endif
00580
00581 #ifdef VERGBOSE_DEBUG
00582 #define ANNOUNCE_FUNCTION
00583     do {
00584         Vnm_printf(2, "%s() [%s:%d]\n",
00585             PRINT_FUNC, __FILE__, __LINE__); \
00586     } while(0)
00587
00588 #define WARN_UNTESTED
00589     do {
00590         Vnm_printf(2, "%s() [%s:%d]: Untested Translation!\n", \
00591             __FUNCTION__, __FILE__, __LINE__); \
00592     } while(0)
00593
00594 #define WARN_PARTTESTED
00595     do{
00596         Vnm_printf(2, "%s() [%s:%d]: Partially Tested Translation.\n", \
00597             __FUNCTION__, __FILE__, __LINE__); \
00598     } while(0)
00599 #else
00600 #define ANNOUNCE_FUNCTION
00601 #define WARN_UNTESTED
00602 #define WARN_PARTTESTED
00603 #endif
00604
00605
00606
00607 /* Utility messages. Print out messages with location information */
00608 #ifdef DEBUG
00609 #define VCHANNELEDMESSAGE0(channel, msg)
00610     do {
00611         Vnm_printf(channel, "%s:%d [%s()]: MESSAGE:\n"
00612             " %s\n\n",
00613             __FILE__, __LINE__, __FUNCTION__, msg); \
00614     } while(0)
00615
00616 #define VCHANNELEDMESSAGE1(channel, msg, arg)
00617     do {
00618         char buff[1000];
00619         snprintf( buff, 1000, msg, arg );
00620         Vnm_printf(channel, "%s:%d [%s()]: MESSAGE:\n"
00621             " %s\n\n",
00622             __FILE__, __LINE__, __FUNCTION__, buff); \
00623     } while(0)
00624
00625 #define VCHANNELEDMESSAGE2(channel, msg, arg0, arg1)
00626     do {
00627         char buff[1000];
00628         snprintf( buff, 1000, msg, arg0, arg1 );
00629         Vnm_printf(channel, "%s:%d [%s()]: MESSAGE:\n"
00630             " %s\n\n",
00631             __FILE__, __LINE__, __FUNCTION__, buff); \
00632     } while(0)
00633
00634 #define VCHANNELEDMESSAGE3(channel, msg, arg0, arg1, arg2)
00635     do {
00636         char buff[1000];
00637         snprintf(buff, 1000, msg, arg0, arg1, arg2);
00638         Vnm_printf(channel, "%s:%d [%s()]: MESSAGE:\n"
00639             " %s\n\n",
00640             __FILE__, __LINE__, __FUNCTION__, buff); \
00641     } while(0)
00642
00643 #define VMESAGE0(msg) VCHANNELEDMESSAGE0(2, msg)
00644 #define VMESAGE1(msg, arg0) VCHANNELEDMESSAGE1(2, msg, arg0)
00645 #define VMESAGE2(msg, arg0, arg1) VCHANNELEDMESSAGE2(2, msg, arg0, arg1)
00646 #define VMESAGE3(msg, arg0, arg1, arg2) VCHANNELEDMESSAGE3(2, msg, arg0, arg1, arg2)
00647
00648 #define VERRMSG0(msg) VMESAGE0(msg)
00649 #define VERRMSG1(msg, arg0) VMESAGE1(msg, arg0)
00650 #define VERRMSG2(msg, arg0, arg1) VMESAGE2(msg, arg0, arg1)
00651 #define VERRMSG3(msg, arg0, arg1, arg2) VMESAGE3(msg, arg0, arg1, arg2)
00652 #else

```

```

00653 #define VCHANNELEDMESSAGE0(channel, msg)          \
00654     do {                                           \
00655         Vnm_print(channel, "%s: %s\n", __FUNCTION__, msg); \
00656     } while(0)
00657
00658 #define VCHANNELEDMESSAGE1(channel, msg, arg0)      \
00659     do {                                           \
00660         char buff[1000];                          \
00661         snprintf( buff, 1000, msg, arg0 );          \
00662         Vnm_print(channel, "%s: %s\n", __FUNCTION__, buff); \
00663     } while(0)
00664
00665 #define VCHANNELEDMESSAGE2(channel, msg, arg0, arg1) \
00666     do {                                           \
00667         char buff[1000];                          \
00668         snprintf( buff, 1000, msg, arg0, arg1 );   \
00669         Vnm_print(channel, "%s: %s\n", __FUNCTION__, buff); \
00670     } while(0)
00671
00672 #define VCHANNELEDMESSAGE3(channel, msg, arg0, arg1, arg2) \
00673     do {                                           \
00674         char buff[1000];                          \
00675         snprintf(buff, 1000, msg, arg0, arg1, arg2); \
00676         Vnm_print(channel, "%s: %s\n", __FUNCTION__, buff); \
00677     } while(0)
00678
00679 #define VMESAGE0(msg) VCHANNELEDMESSAGE0(0, msg)
00680 #define VMESAGE1(msg, arg0) VCHANNELEDMESSAGE1(0, msg, arg0)
00681 #define VMESAGE2(msg, arg0, arg1) VCHANNELEDMESSAGE2(0, msg, arg0, arg1)
00682 #define VMESAGE3(msg, arg0, arg1, arg2) VCHANNELEDMESSAGE3(0, msg, arg0, arg1, arg2)
00683
00684 #define VERRMSG0(msg) VCHANNELEDMESSAGE0(2, msg)
00685 #define VERRMSG1(msg, arg0) VCHANNELEDMESSAGE1(2, msg, arg0)
00686 #define VERRMSG2(msg, arg0, arg1) VCHANNELEDMESSAGE2(2, msg, arg0, arg1)
00687 #define VERRMSG3(msg, arg0, arg1, arg2) VCHANNELEDMESSAGE3(2, msg, arg0, arg1, arg2)
00688 #endif
00689
00690
00691
00692 /* Utility assertions. If they fail, they print out messages with possible
00693  * arguments and then abort
00694  * The do{...} while(0) simply enforces that a semicolon appears at the end
00695  */
00696 #ifdef DEBUG
00697 #define VASSERT_MSG0(cnd, msg) \
00698     do { \
00699         if( (cnd) == 0 ) { \
00700             Vnm_print(2, "%s:%d [%s()]: ERROR:\n" \
00701                 "    Assertion Failed (%s): %s\n\n", \
00702                 __FILE__, __LINE__, __FUNCTION__, #cnd, msg); \
00703             abort(); \
00704         } \
00705     } while(0)
00706
00707 #define VASSERT_MSG1(cnd, msg, arg) \
00708     do { \
00709         if( (cnd) == 0 ) { \
00710             char buff[1000]; \
00711             snprintf( buff, 1000, msg, arg ); \
00712             Vnm_print(2, "%s:%d [%s()]: ERROR:\n" \
00713                 "    Assertion Failed (%s): %s\n\n", \
00714                 __FILE__, __LINE__, __FUNCTION__, #cnd, buff); \
00715             abort(); \
00716         } \
00717     } while(0)
00718
00719 #define VASSERT_MSG2(cnd, msg, arg0, arg1) \
00720     do { \
00721         if( (cnd) == 0 ) { \
00722             char buff[1000]; \
00723             snprintf( buff, 1000, msg, arg0, arg1 ); \
00724             Vnm_print(2, "%s:%d [%s()]: ERROR:\n" \
00725                 "    Assertion Failed (%s): %s\n\n", \
00726                 __FILE__, __LINE__, __FUNCTION__, #cnd, buff); \
00727             abort(); \
00728         } \
00729     } while(0)
00730 #else
00731 #define VASSERT_MSG0(cnd, msg) \
00732     do { \
00733         if( (cnd) == 0 ) { \

```

```

00734         Vnm_print(2, "[%s()]: ERROR:\n"
00735             "        Assertion Failed (%s): %s\n\n",
00736             __FUNCTION__, #cnd, msg);
00737         abort();
00738     }
00739 } while(0)
00740
00741 #define VASSERT_MSG1(cnd, msg, arg)
00742 do {
00743     if( (cnd) == 0 ) {
00744         char buff[1000];
00745         snprintf( buff, 1000, msg, arg );
00746         Vnm_print(2, "[%s()]: ERROR:\n"
00747             "        Assertion Failed (%s): %s\n\n",
00748             __FUNCTION__, #cnd, buff);
00749         abort();
00750     }
00751 } while(0)
00752
00753 #define VASSERT_MSG2(cnd, msg, arg0, arg1)
00754 do {
00755     if( (cnd) == 0 ) {
00756         char buff[1000];
00757         snprintf( buff, 1000, msg, arg0, arg1 );
00758         Vnm_print(2, "[%s()]: ERROR:\n"
00759             "        Assertion Failed (%s): %s\n\n",
00760             __FUNCTION__, #cnd, buff);
00761         abort();
00762     }
00763 } while(0)
00764 #endif
00765
00766
00767
00768 /* Utility warning. Tests a condition and if it fails prints out a message
00769  * with optional arguments
00770  * The do{...} while(0) simply enforces that a semicolon at the end
00771  */
00772 #ifdef DEBUG
00773 #define VWARN_MSG0(cnd, msg)
00774 do {
00775     if( (cnd) == 0 ) {
00776         Vnm_print(
00777             2,
00778             "%s:%d [%s()]: WARNING:\n"
00779             "        Condition Failed (%s):\n    %s\n\n",
00780             __FILE__,
00781             __LINE__,
00782             __FUNCTION__,
00783             #cnd,
00784             msg
00785             );
00786     }
00787 } while(0)
00788
00789 #define VWARN_MSG1(cnd, msg, arg0)
00790 do {
00791     if( (cnd) == 0 ) {
00792         char buff[1000];
00793         snprintf(buff, 1000, msg, arg0);
00794         Vnm_print(
00795             2,
00796             "%s:%d [%s()]: WARNING:\n"
00797             "        Condition Failed (%s):\n    %s\n\n",
00798             __FILE__,
00799             __LINE__,
00800             __FUNCTION__,
00801             #cnd,
00802             buff
00803             );
00804     }
00805 } while(0)
00806
00807 #define VWARN_MSG2(cnd, msg, arg0, arg1)
00808 do {
00809     if( (cnd) == 0 ) {
00810         char buff[1000];
00811         snprintf(buff, 1000, msg, arg0, arg1);
00812         Vnm_print(
00813             2,
00814             "%s:%d [%s()]: WARNING:\n"

```

```

00815             "    Condition Failed (%s):\n    %s\n\n", \
00816             __FILE__, \
00817             __LINE__, \
00818             __FUNCTION__, \
00819             #cnd, \
00820             buff \
00821             ); \
00822         } \
00823     } while(0) \
00824 #else \
00825 #define VWARN_MSG0(cnd, msg) \
00826     do { \
00827         if( (cnd) == 0 ) { \
00828             Vnm_print( \
00829                 2, \
00830                 "[%s()]: WARNING:\n" \
00831                 "%s\n\n", \
00832                 __FUNCTION__, \
00833                 msg \
00834                 ); \
00835         } \
00836     } while(0) \
00837 \
00838 #define VWARN_MSG1(cnd, msg, arg0) \
00839     do { \
00840         if( (cnd) == 0 ) { \
00841             char buff[1000]; \
00842             snprintf(buff, 1000, msg, arg0); \
00843             Vnm_print( \
00844                 2, \
00845                 "[%s()]: WARNING:\n" \
00846                 "%s\n\n", \
00847                 __FUNCTION__, \
00848                 buff \
00849                 ); \
00850         } \
00851     } while(0) \
00852 \
00853 #define VWARN_MSG2(cnd, msg, arg0, arg1) \
00854     do { \
00855         if( (cnd) == 0 ) { \
00856             char buff[1000]; \
00857             snprintf(buff, 1000, msg, arg0, arg1); \
00858             Vnm_print( \
00859                 2, \
00860                 "[%s()]: WARNING:\n" \
00861                 "%s\n\n", \
00862                 __FUNCTION__, \
00863                 buff \
00864                 ); \
00865         } \
00866     } while(0) \
00867 #endif \
00868 \
00869 /* Utility Abort. Prints a message with optional arguments and aborts */ \
00870 #ifdef DEBUG \
00871 #define VABORT_MSG0(msg) \
00872     do { \
00873         Vnm_print(2, "%s:%d [%s()]: ABORTING:\n" \
00874                 "%s\n\n", \
00875                 __FILE__, __LINE__, __FUNCTION__, msg); \
00876         abort(); \
00877     } while(0) \
00878 \
00879 #define VABORT_MSG1(msg, arg) \
00880     do { \
00881         char buff[1000]; \
00882         snprintf( buff, 1000, msg, arg ); \
00883         Vnm_print(2, "%s:%d [%s()]: ABORTING:\n" \
00884                 "%s\n\n", \
00885                 __FILE__, __LINE__, __FUNCTION__, buff); \
00886         abort(); \
00887     } while(0) \
00888 \
00889 #define VABORT_MSG2(msg, arg0, arg1) \
00890     do { \
00891         char buff[1000]; \
00892         snprintf( buff, 1000, msg, arg0, arg1); \
00893         Vnm_print(2, "%s:%d [%s()]: ABORTING:\n" \
00894                 "%s\n\n", \
00895                 __FILE__, __LINE__, __FUNCTION__, buff); \

```



```

00896         abort();
00897     } while(0)
00898 #else
00899 #define VABORT_MSG0(msg)
00900     do {
00901         Vnm_print(2, "[%s()]: ABORTING:\n"
00902             "    %s\n\n",
00903             __FUNCTION__, msg);
00904         abort();
00905     } while(0)
00906
00907 #define VABORT_MSG1(msg, arg)
00908     do {
00909         char buff[1000];
00910         snprintf( buff, 1000, msg, arg );
00911         Vnm_print(2, "[%s()]: ABORTING:\n"
00912             "    %s\n\n",
00913             __FUNCTION__, buff);
00914         abort();
00915     } while(0)
00916
00917 #define VABORT_MSG2(msg, arg0, arg1)
00918     do {
00919         char buff[1000];
00920         snprintf( buff, 1000, msg, arg0, arg1);
00921         Vnm_print(2, "[%s()]: ABORTING:\n"
00922             "    %s\n\n",
00923             __FUNCTION__, buff);
00924         abort();
00925     } while(0)
00926 #endif
00927
00928
00929
00930 /* Utility expression printers. Print the expression and its value */
00931 #ifdef DEBUG
00932 #define PRINT_INT(expr)
00933     do {
00934         Vnm_print(2, "%s:%d [%s()]: %s == %d\n",
00935             __FILE__, __LINE__, __FUNCTION__, #expr, expr);
00936     } while(0)
00937
00938 #define PRINT_DBL(expr)
00939     do {
00940         Vnm_print(2, "%s:%d [%s()]: %s == %f\n\n",
00941             __FILE__, __LINE__, __FUNCTION__, #expr, expr);
00942     } while(0)
00943 #else
00944 #define PRINT_INT(expr)
00945 #define PRINT_DBL(expr)
00946 #endif
00947
00948 #define VMALLOC(vmem, n, type) ((type*)Vmem_malloc(vmem, n, sizeof(type)))
00949
00950 #define VFREE(vmem, n, type, ptr) (Vmem_free(vmem, n, sizeof(type), (void **)&(ptr)))
00951
00952 #define VFILL(vec, n, val)
00953     do {
00954         int fill_idx;
00955         for (fill_idx = 0; fill_idx < n; fill_idx++)
00956             vec[fill_idx] = val;
00957     } while(0)
00958
00959 #define VCOPY(srcvec, dstvec, i, n)
00960     do {
00961         for (i = 0; i < n; i++)
00962             dstvec[i] = srcvec[i];
00963     } while(0)
00964
00965
00966 char* wrap_text( char* str, int right_margin, int left_padding );
00967
00968 #define VAT(array, i) ((array)[(i) - 1])
00969 #define RAT(array, i) ((array) + i - 1)
00970
00971 #endif /* #ifndef _VAPBSHAL_H_ */

```



```

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*

```

Definition in file [vmatrix.h](#).

9.76.2 Macro Definition Documentation

9.76.2.1 MAT2

```

#define MAT2(
    mat,
    dx,
    dy )

```

Value:

```

    int dx_##mat = dx;    \
    int dy_##mat = dy

```

Definition at line 64 of file [vmatrix.h](#).

9.76.2.2 MAT3

```

#define MAT3(
    mat,
    dx,
    dy,
    dz )

```

Value:

```

    int dx_##mat = dx;    \
    int dy_##mat = dy;    \
    int dz_##mat = dz

```

Definition at line 76 of file [vmatrix.h](#).

9.76.2.3 RAT2

```

#define RAT2(
    mat,

```

```

    x,
    y ) &VAT2(mat, x, y)

```

Definition at line 68 of file [vmatrix.h](#).

9.76.2.4 RAT3

```

#define RAT3(
    mat,
    x,
    y,
    z ) &VAT3(mat, x, y, z)

```

Definition at line 81 of file [vmatrix.h](#).

9.76.2.5 VAT2

```

#define VAT2(
    mat,
    x,
    y ) mat[(y - 1) * dx_##mat + (x - 1)]

```

Definition at line 71 of file [vmatrix.h](#).

9.76.2.6 VAT3

```

#define VAT3(
    mat,
    x,
    y,
    z )

```

Value:

```

    mat[(z - 1) * dy_##mat * dx_##mat + \
        (y - 1) * dx_##mat + \
        (x - 1)]

```

Definition at line 84 of file [vmatrix.h](#).

9.77 vmatrix.h

[Go to the documentation of this file.](#)

```

00001
00061 #ifndef _VMATRIX_H_
00062 #define _VMATRIX_H_
00063
00064 #define MAT2(mat, dx, dy) \
00065     int dx_##mat = dx; \
00066     int dy_##mat = dy
00067
00068 #define RAT2(mat, x, y) \
00069     &VAT2(mat, x, y)
00070
00071 #define VAT2(mat, x, y) \
00072     mat[(y - 1) * dx_##mat + (x - 1)]
00073
00074
00075
00076 #define MAT3(mat, dx, dy, dz) \
00077     int dx_##mat = dx; \
00078     int dy_##mat = dy; \
00079     int dz_##mat = dz
00080
00081 #define RAT3(mat, x, y, z) \
00082     &VAT3(mat, x, y, z)
00083
00084 #define VAT3(mat, x, y, z) \
00085     mat[(z - 1) * dy_##mat * dx_##mat + \
00086         (y - 1) * dx_##mat + \

```

```

00087         (x - 1)]
00088
00089 #endif /* _VMATRIX_H_ */

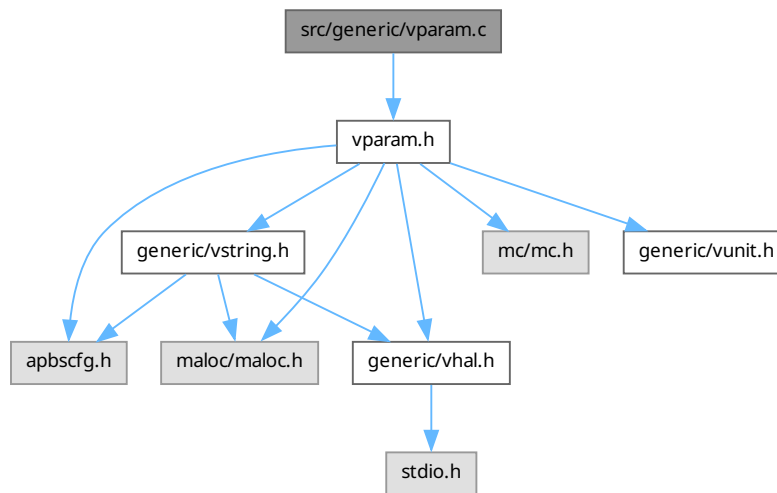
```

9.78 src/generic/vparam.c File Reference

Class [Vparam](#) methods.

```
#include "vparam.h"
```

Include dependency graph for vparam.c:



Functions

- VPRIVATE int [readFlatFileLine](#) (Vio *sock, [Vparam_AtomData](#) *atom)
Read a single line of the flat file database.
- VPRIVATE int [readXMLFileAtom](#) (Vio *sock, [Vparam_AtomData](#) *atom)
Read atom information from an XML file.
- VPUBLIC unsigned long int [Vparam_memChk](#) ([Vparam](#) *thee)
Get number of bytes in this object and its members.
- VPUBLIC [Vparam_AtomData](#) * [Vparam_AtomData_ctor](#) ()
Construct the object.
- VPUBLIC int [Vparam_AtomData_ctor2](#) ([Vparam_AtomData](#) *thee)
FORTTRAN stub to construct the object.
- VPUBLIC void [Vparam_AtomData_dtor](#) ([Vparam_AtomData](#) **thee)
Destroy object.
- VPUBLIC void [Vparam_AtomData_dtor2](#) ([Vparam_AtomData](#) *thee)
FORTTRAN stub to destroy object.
- VPUBLIC [Vparam_ResData](#) * [Vparam_ResData_ctor](#) (Vmem *mem)
Construct the object.
- VPUBLIC int [Vparam_ResData_ctor2](#) ([Vparam_ResData](#) *thee, Vmem *mem)
FORTTRAN stub to construct the object.

- VPUBLIC void `Vparam_ResData_dtor` (`Vparam_ResData **thee`)
Destroy object.
- VPUBLIC void `Vparam_ResData_dtor2` (`Vparam_ResData *thee`)
FORTTRAN stub to destroy object.
- VPUBLIC `Vparam * Vparam_ctor` ()
Construct the object.
- VPUBLIC int `Vparam_ctor2` (`Vparam *thee`)
FORTTRAN stub to construct the object.
- VPUBLIC void `Vparam_dtor` (`Vparam **thee`)
Destroy object.
- VPUBLIC void `Vparam_dtor2` (`Vparam *thee`)
FORTTRAN stub to destroy object.
- VPUBLIC `Vparam_ResData * Vparam_getResData` (`Vparam *thee`, char resName[VMAX_ARGLEN])
Get residue data.
- VPUBLIC `Vparam_AtomData * Vparam_getAtomData` (`Vparam *thee`, char resName[VMAX_ARGLEN], char atomName[VMAX_ARGLEN])
Get atom data.
- VPUBLIC int `Vparam_readXMLFile` (`Vparam *thee`, const char *iodev, const char *iofmt, const char *thost, const char *fname)
Read an XML format parameter database.
- VPUBLIC int `Vparam_readFlatFile` (`Vparam *thee`, const char *iodev, const char *iofmt, const char *thost, const char *fname)
Read a flat-file format parameter database.
- VEXTERNC void `Vparam_AtomData_copyTo` (`Vparam_AtomData *thee`, `Vparam_AtomData *dest`)
Copy current atom object to destination.
- VEXTERNC void `Vparam_ResData_copyTo` (`Vparam_ResData *thee`, `Vparam_ResData *dest`)
Copy current residue object to destination.
- VEXTERNC void `Vparam_AtomData_copyFrom` (`Vparam_AtomData *thee`, `Vparam_AtomData *src`)
Copy current atom object from another.

Variables

- VPRIVATE char * `MCwhiteChars` = " =,;\t\n\r"
Whitespace characters for socket reads.
- VPRIVATE char * `MCcommChars` = "#%"
Comment characters for socket reads.
- VPRIVATE char * `MCxmlwhiteChars` = " =,;\t\n\r<>"
Whitespace characters for XML socket reads.

9.78.1 Detailed Description

Class `Vparam` methods.

Author

Nathan Baker

Version

\$Id\$

Attention

```

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*
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*
*

```

Definition in file [vparam.c](#).

9.79 vparam.c

[Go to the documentation of this file.](#)

```

00001
00057 #include "vparam.h"
00058
00059 VEMBED(rcsid="$Id$")
00060
00061
00065 VPRIVATE char *MCwhiteChars = " =,;\t\n\r";
00066
00071 VPRIVATE char *MCcommChars = "#%";
00072
00077 VPRIVATE char *MCxmlwhiteChars = " =,;\t\n\r<>";
00078
00087 VPRIVATE int readFlatFileLine(Vio *sock, Vparam_AtomData *atom);
00088
00097 VPRIVATE int readXMLFileAtom(Vio *sock, Vparam_AtomData *atom);

```

```

00098
00099
00100 #if !defined(VINLINE_VPARAM)
00101
00102 VPUBLIC unsigned long int Vparam_memChk(Vparam *thee) {
00103     if (thee == VNULL) return 0;
00104     return Vmem_bytes(thee->vmem);
00105 }
00106
00107 #endif /* if !defined(VINLINE_VPARAM) */
00108
00109 VPUBLIC Vparam_AtomData* Vparam_AtomData_ctor() {
00110     Vparam_AtomData *thee = VNULL;
00111
00112     /* Set up the structure */
00113     thee = (Vparam_AtomData*)Vmem_malloc(VNULL, 1, sizeof(Vparam_AtomData) );
00114     VASSERT(thee != VNULL);
00115     VASSERT(Vparam_AtomData_ctor2(thee));
00116
00117     return thee;
00118 }
00119
00120
00121 VPUBLIC int Vparam_AtomData_ctor2(Vparam_AtomData *thee) { return 1; }
00122
00123 VPUBLIC void Vparam_AtomData_dtor(Vparam_AtomData **thee) {
00124
00125     if ((*thee) != VNULL) {
00126         Vparam_AtomData_dtor2(*thee);
00127         Vmem_free(VNULL, 1, sizeof(Vparam_AtomData), (void **)thee);
00128         (*thee) = VNULL;
00129     }
00130
00131 }
00132
00133 VPUBLIC void Vparam_AtomData_dtor2(Vparam_AtomData *thee) { ; }
00134
00135 VPUBLIC Vparam_ResData* Vparam_ResData_ctor(Vmem *mem) {
00136
00137     Vparam_ResData *thee = VNULL;
00138
00139     /* Set up the structure */
00140     thee = (Vparam_ResData*)Vmem_malloc(mem, 1, sizeof(Vparam_ResData) );
00141     VASSERT(thee != VNULL);
00142     VASSERT(Vparam_ResData_ctor2(thee, mem));
00143
00144     return thee;
00145 }
00146
00147 VPUBLIC int Vparam_ResData_ctor2(Vparam_ResData *thee, Vmem *mem) {
00148
00149     if (thee == VNULL) {
00150         Vnm_print(2, "Vparam_ResData_ctor2: Got VNULL thee!\n");
00151         return 0;
00152     }
00153     thee->vmem = mem;
00154     thee->nAtomData = 0;
00155     thee->atomData = VNULL;
00156
00157     return 1;
00158 }
00159
00160 VPUBLIC void Vparam_ResData_dtor(Vparam_ResData **thee) {
00161
00162     if ((*thee) != VNULL) {
00163         Vparam_ResData_dtor2(*thee);
00164         Vmem_free((*thee)->vmem, 1, sizeof(Vparam_ResData), (void **)thee);
00165         (*thee) = VNULL;
00166     }
00167
00168 }
00169
00170 VPUBLIC void Vparam_ResData_dtor2(Vparam_ResData *thee) {
00171
00172     if (thee == VNULL) return;
00173     if (thee->nAtomData > 0) {
00174         Vmem_free(thee->vmem, thee->nAtomData, sizeof(Vparam_AtomData),
00175             (void **)&(thee->atomData));
00176     }
00177     thee->nAtomData = 0;
00178     thee->atomData = VNULL;

```



```

00179 }
00180
00181 VPUBLIC Vparam* Vparam_ctor() {
00182     Vparam *thee = VNULL;
00183
00184     /* Set up the structure */
00185     thee = (Vparam*)Vmem_malloc(VNULL, 1, sizeof(Vparam));
00186     VASSERT(thee != VNULL);
00187     VASSERT(Vparam_ctor2(thee));
00188
00189     return thee;
00190 }
00191
00192
00193 VPUBLIC int Vparam_ctor2(Vparam *thee) {
00194     if (thee == VNULL) {
00195         Vnm_print(2, "Vparam_ctor2: got VNULL thee!\n");
00196         return 0;
00197     }
00198
00199     thee->vmem = VNULL;
00200     thee->vmem = Vmem_ctor("APBS:VPARAM");
00201     if (thee->vmem == VNULL) {
00202         Vnm_print(2, "Vparam_ctor2: failed to init Vmem!\n");
00203         return 0;
00204     }
00205
00206     thee->nResData = 0;
00207     thee->resData = VNULL;
00208
00209     return 1;
00210 }
00211
00212
00213 VPUBLIC void Vparam_dtor(Vparam **thee) {
00214     if ((*thee) != VNULL) {
00215         Vparam_dtor2(*thee);
00216         Vmem_free(VNULL, 1, sizeof(Vparam), (void **)thee);
00217         (*thee) = VNULL;
00218     }
00219 }
00220
00221 }
00222
00223 VPUBLIC void Vparam_dtor2(Vparam *thee) {
00224     int i;
00225
00226     if (thee == VNULL) return;
00227
00228     /* Destroy the residue data */
00229     for (i=0; i<thee->nResData; i++) Vparam_ResData_dtor2(&(thee->resData[i]));
00230     if (thee->nResData > 0) Vmem_free(thee->vmem, thee->nResData,
00231         sizeof(Vparam_ResData), (void **)&(thee->resData));
00232     thee->nResData = 0;
00233     thee->resData = VNULL;
00234
00235     if (thee->vmem != VNULL) Vmem_dtor(&(thee->vmem));
00236     thee->vmem = VNULL;
00237
00238 }
00239
00240
00241 VPUBLIC Vparam_ResData* Vparam_getResData(Vparam *thee,
00242     char resName[VMAX_ARGLEN]) {
00243     int i;
00244     Vparam_ResData *res = VNULL;
00245
00246     VASSERT(thee != VNULL);
00247
00248     if ((thee->nResData == 0) || (thee->resData == VNULL)) {
00249         res = VNULL;
00250         return res;
00251     }
00252
00253     /* Look for the matching residue */
00254     for (i=0; i<thee->nResData; i++) {
00255         res = &(thee->resData[i]);
00256         if (Vstring_strcasecmp(resName, res->name) == 0) return res;
00257     }
00258 }
00259

```

```

00260
00261     /* Didn't find a matching residue */
00262     res = VNULL;
00263     Vnm_print(2, "Vparam_getResData: unable to find res=%s\n", resName);
00264     return res;
00265 }
00266
00267 VPUBLIC Vparam_AtomData* Vparam_getAtomData(Vparam *thee,
00268     char resName[VMAX_ARGLEN], char atomName[VMAX_ARGLEN]) {
00269     int i;
00270     Vparam_ResData *res = VNULL;
00271     Vparam_AtomData *atom = VNULL;
00272
00273     VASSERT(thee != VNULL);
00274
00275     if ((thee->nResData == 0) || (thee->resData == VNULL)) {
00276         atom = VNULL;
00277         return atom;
00278     }
00279
00280     /* Look for the matching residue */
00281     res = Vparam_getResData(thee, resName);
00282     if (res == VNULL) {
00283         atom = VNULL;
00284         Vnm_print(2, "Vparam_getAtomData: Unable to find residue %s!\n", resName);
00285         return atom;
00286     }
00287
00288     for (i=0; i<res->nAtomData; i++) {
00289         atom = &(res->atomData[i]);
00290         if (atom == VNULL) {
00291             Vnm_print(2, "Vparam_getAtomData: got NULL atom!\n");
00292             return VNULL;
00293         }
00294         if (Vstring_strcasecmp(atomName, atom->atomName) == 0) {
00295             return atom;
00296         }
00297     }
00298
00299     /* Didn't find a matching atom/residue */
00300     atom = VNULL;
00301     Vnm_print(2, "Vparam_getAtomData: unable to find atom '%s', res '%s'\n",
00302         atomName, resName);
00303     return atom;
00304 }
00305
00306 VPUBLIC int Vparam_readXMLFile(Vparam *thee, const char *iodev,
00307     const char *iofmt, const char *thost, const char *fname) {
00308
00309     int i, ires, natoms, nalloc, ralloc;
00310     Vparam_AtomData *atoms = VNULL;
00311     Vparam_AtomData *tatoms = VNULL;
00312     Vparam_AtomData *atom = VNULL;
00313     Vparam_ResData *res = VNULL;
00314     Vparam_ResData *residues = VNULL;
00315     Vparam_ResData *tresidues = VNULL;
00316     Vio *sock = VNULL;
00317     char currResName[VMAX_ARGLEN];
00318     char tok[VMAX_ARGLEN];
00319     char endtag[VMAX_ARGLEN];
00320
00321     VASSERT(thee != VNULL);
00322
00323     /* Setup communication */
00324     sock = Vio_ctor(iodev, iofmt, thost, fname, "r");
00325     if (sock == VNULL) {
00326         Vnm_print(2, "Vparam_readXMLFile: Problem opening virtual socket %s\n",
00327             fname);
00328         return 0;
00329     }
00330     if (Vio_accept(sock, 0) < 0) {
00331         Vnm_print(2, "Vparam_readXMLFile: Problem accepting virtual socket %s\n",
00332             fname);
00333         return 0;
00334     }
00335     Vio_setWhiteChars(sock, MCxmlwhiteChars);
00336     Vio_setCommChars(sock, MCcommChars);
00337
00338     /* Clear existing parameters */
00339     if (thee->nResData > 0) {
00340         Vnm_print(2, "WARNING -- CLEARING PARAMETER DATABASE!\n");

```

```

00341         for (i=0; i<thee->nResData; i++) {
00342             Vparam_ResData_dtor2(&(thee->resData[i]));
00343         }
00344         Vmem_free(thee->vmem, thee->nResData,
00345             sizeof(Vparam_ResData), (void *)&(thee->resData));
00346     }
00347     strcpy(endtag, "/");
00348
00349     /* Set up temporary residue list */
00350
00351     ralloc = 50;
00352     residues = (Vparam_ResData*)Vmem_malloc(thee->vmem, ralloc, sizeof(Vparam_ResData));
00353
00354     /* Read until we run out of entries, allocating space as needed */
00355     while (1) {
00356         VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00357
00358         /* The first token should be the start tag */
00359
00360         if (Vstring_strcasecmp(endtag, "/") == 0) strcat(endtag, tok);
00361
00362         if (Vstring_strcasecmp(tok, "residue") == 0) {
00363             if (thee->nResData >= ralloc) {
00364                 tresidues = (Vparam_ResData*)Vmem_malloc(thee->vmem, 2*ralloc, sizeof(Vparam_ResData));
00365                 VASSERT(tresidues != VNULL);
00366                 for (i=0; i<thee->nResData; i++) {
00367                     Vparam_ResData_copyTo(&(residues[i]), &(tresidues[i]));
00368                 }
00369                 Vmem_free(thee->vmem, ralloc, sizeof(Vparam_ResData),
00370                     (void *)&(residues));
00371                 residues = tresidues;
00372                 tresidues = VNULL;
00373                 ralloc = 2*ralloc;
00374             }
00375
00376             /* Initial space for this residue's atoms */
00377             nalloc = 20;
00378             natoms = 0;
00379             atoms = (Vparam_AtomData*)Vmem_malloc(thee->vmem, nalloc, sizeof(Vparam_AtomData));
00380
00381             } else if (Vstring_strcasecmp(tok, "name") == 0) {
00382                 VJMPERR1(Vio_scanf(sock, "%s", tok) == 1); /* value */
00383                 strcpy(currResName, tok);
00384                 VJMPERR1(Vio_scanf(sock, "%s", tok) == 1); /* </name> */
00385             } else if (Vstring_strcasecmp(tok, "atom") == 0) {
00386                 if (natoms >= nalloc) {
00387                     tatoms = (Vparam_AtomData*)Vmem_malloc(thee->vmem, 2*nalloc, sizeof(Vparam_AtomData));
00388                     VASSERT(tatoms != VNULL);
00389                     for (i=0; i<natoms; i++) {
00390                         Vparam_AtomData_copyTo(&(atoms[i]), &(tatoms[i]));
00391                     }
00392                     Vmem_free(thee->vmem, nalloc, sizeof(Vparam_AtomData),
00393                         (void *)&(atoms));
00394                     atoms = tatoms;
00395                     tatoms = VNULL;
00396                     nalloc = 2*nalloc;
00397                 }
00398                 atom = &(atoms[natoms]);
00399                 if (!readXMLFileAtom(sock, atom)) break;
00400                 natoms++;
00401             } else if (Vstring_strcasecmp(tok, "/residue") == 0) {
00402                 res = &(residues[thee->nResData]);
00403                 Vparam_ResData_ctor2(res, thee->vmem);
00404                 res->atomData = (Vparam_AtomData*)Vmem_malloc(thee->vmem, natoms,
00405                     sizeof(Vparam_AtomData));
00406                 res->nAtomData = natoms;
00407                 strcpy(res->name, currResName);
00408                 for (i=0; i<natoms; i++) {
00409                     strcpy(atoms[i].resName, currResName);
00410                     Vparam_AtomData_copyTo(&(atoms[i]), &(res->atomData[i]));
00411                 }
00412                 Vmem_free(thee->vmem, nalloc, sizeof(Vparam_AtomData), (void *)&(atoms));
00413                 (thee->nResData)++;
00414             } else if (Vstring_strcasecmp(tok, endtag) == 0) break;
00415         }
00416     }
00417 }
00418
00419
00420
00421

```

```

00422     /* Initialize and copy the residues into the Vparam object */
00423
00424     thee->resData = (Vparam_ResData*)Vmem_malloc(thee->vmem, thee->nResData,
00425         sizeof(Vparam_ResData));
00426     for (ires=0; ires<thee->nResData; ires++) {
00427         Vparam_ResData_copyTo(&(residues[ires]), &(thee->resData[ires]));
00428     }
00429
00430     /* Destroy temporary atom space */
00431     Vmem_free(thee->vmem, ralloc, sizeof(Vparam_ResData), (void **)&(residues));
00432
00433     /* Shut down communication */
00434     Vio_acceptFree(sock);
00435     Vio_dtor(&sock);
00436
00437     return 1;
00438
00439 ERROR1:
00440     Vnm_print(2, "Vparam_readXMLFile: Got unexpected EOF reading parameter file!\n");
00441     return 0;
00442
00443 }
00444
00445 VPUBLIC int Vparam_readFlatFile(Vparam *thee, const char *iodev,
00446     const char *iofmt, const char *thost, const char *fname) {
00447
00448     int i, iatom, jatom, ires, natoms, nalloc;
00449     Vparam_AtomData *atoms = VNULL;
00450     Vparam_AtomData *tatoms = VNULL;
00451     Vparam_AtomData *atom = VNULL;
00452     Vparam_ResData *res = VNULL;
00453     Vio *sock = VNULL;
00454     char currResName[VMAX_ARGLEN];
00455
00456     VASSERT(thee != VNULL);
00457
00458     /* Setup communication */
00459     sock = Vio_ctor(iodev, iofmt, thost, fname, "r");
00460     if (sock == VNULL) {
00461         Vnm_print(2, "Vparam_readFlatFile: Problem opening virtual socket %s\n",
00462             fname);
00463         return 0;
00464     }
00465     if (Vio_accept(sock, 0) < 0) {
00466         Vnm_print(2, "Vparam_readFlatFile: Problem accepting virtual socket %s\n",
00467             fname);
00468         return 0;
00469     }
00470     Vio_setWhiteChars(sock, MCwhiteChars);
00471     Vio_setCommChars(sock, MCcommChars);
00472
00473     /* Clear existing parameters */
00474     if (thee->nResData > 0) {
00475         Vnm_print(2, "WARNING -- CLEARING PARAMETER DATABASE!\n");
00476         for (i=0; i<thee->nResData; i++) {
00477             Vparam_ResData_dtor2(&(thee->resData[i]));
00478         }
00479         Vmem_free(thee->vmem, thee->nResData,
00480             sizeof(Vparam_ResData), (void **)&(thee->resData));
00481     }
00482
00483     /* Initial space for atoms */
00484     nalloc = 200;
00485     natoms = 0;
00486     atoms = (Vparam_AtomData*)Vmem_malloc(thee->vmem, nalloc, sizeof(Vparam_AtomData));
00487
00488     /* Read until we run out of entries, allocating space as needed */
00489     while (1) {
00490         if (natoms >= nalloc) {
00491             tatoms = (Vparam_AtomData*)Vmem_malloc(thee->vmem, 2*nalloc, sizeof(Vparam_AtomData));
00492             VASSERT(tatoms != VNULL);
00493             for (i=0; i<natoms; i++) {
00494                 Vparam_AtomData_copyTo(&(atoms[i]), &(tatoms[i]));
00495             }
00496             Vmem_free(thee->vmem, nalloc, sizeof(Vparam_AtomData),
00497                 (void **)&(atoms));
00498             atoms = tatoms;
00499             tatoms = VNULL;
00500             nalloc = 2*nalloc;
00501         }
00502         atom = &(atoms[natoms]);

```

```

00503         if (!readFlatFileLine(sock, atom)) break;
00504         natoms++;
00505     }
00506     if (natoms == 0) return 0;
00507
00508     /* Count the number of residues */
00509     thee->nResData = 1;
00510     strcpy(currResName, atoms[0].resName);
00511     for (i=1; i<natoms; i++) {
00512         if (Vstring_strcasecmp(atoms[i].resName, currResName) != 0) {
00513             strcpy(currResName, atoms[i].resName);
00514             (thee->nResData)++;
00515         }
00516     }
00517
00518     /* Create the residues */
00519     thee->resData = (Vparam_ResData*)Vmem_malloc(thee->vmem, thee->nResData,
00520         sizeof(Vparam_ResData));
00521     VASSERT(thee->resData != VNULL);
00522     for (i=0; i<(thee->nResData); i++) {
00523         res = &(thee->resData[i]);
00524         Vparam_ResData_ctor2(res, thee->vmem);
00525     }
00526
00527     /* Count the number of atoms per residue */
00528     ires = 0;
00529     res = &(thee->resData[ires]);
00530     res->nAtomData = 1;
00531     strcpy(res->name, atoms[0].resName);
00532     for (i=1; i<natoms; i++) {
00533         if (Vstring_strcasecmp(atoms[i].resName, res->name) != 0) {
00534             (ires)++;
00535             res = &(thee->resData[ires]);
00536             res->nAtomData = 1;
00537             strcpy(res->name, atoms[i].resName);
00538         } else (res->nAtomData)++;
00539     }
00540
00541     /* Allocate per-residue space for atoms */
00542     for (ires=0; ires<thee->nResData; ires++) {
00543         res = &(thee->resData[ires]);
00544         res->atomData = (Vparam_AtomData*)Vmem_malloc(thee->vmem, res->nAtomData,
00545             sizeof(Vparam_AtomData));
00546     }
00547
00548     /* Copy atoms into residues */
00549     iatom = 0;
00550     Vparam_AtomData_copyTo(&(atoms[0]), &(res->atomData[iatom]));
00551     for (ires=0; ires<thee->nResData; ires++) {
00552         res = &(thee->resData[ires]);
00553         for (jatom=0; jatom<res->nAtomData; jatom++) {
00554             Vparam_AtomData_copyTo(&(atoms[iatom]), &(res->atomData[jatom]));
00555             iatom++;
00556         }
00557     }
00558
00559
00560     /* Shut down communication */
00561     Vio_acceptFree(sock);
00562     Vio_dtor(&sock);
00563
00564     /* Destroy temporary atom space */
00565     Vmem_free(thee->vmem, nalloc, sizeof(Vparam_AtomData), (void **)&(atoms));
00566
00567     return 1;
00568
00569 }
00570
00571 VEXTERNC void Vparam_AtomData_copyTo(Vparam_AtomData *thee,
00572     Vparam_AtomData *dest) {
00573
00574     VASSERT(thee != VNULL);
00575     VASSERT(dest != VNULL);
00576
00577     strcpy(dest->atomName, thee->atomName);
00578     strcpy(dest->resName, thee->resName);
00579     dest->charge = thee->charge;
00580     dest->radius = thee->radius;
00581     dest->epsilon = thee->epsilon;
00582
00583 }

```

```

00584
00585 VEXTERNC void Vparam_ResData_copyTo(Vparam_ResData *thee,
00586   Vparam_ResData *dest) {
00587
00588     int i;
00589
00590     VASSERT(thee != VNULL);
00591     VASSERT(dest != VNULL);
00592
00593     strcpy(dest->name, thee->name);
00594     dest->vmem = thee->vmem;
00595     dest->nAtomData = thee->nAtomData;
00596
00597     dest->atomData = (Vparam_AtomData*)Vmem_malloc(thee->vmem, dest->nAtomData,
00598       sizeof(Vparam_AtomData));
00599
00600     for (i=0; i<dest->nAtomData; i++) {
00601       Vparam_AtomData_copyTo(&(thee->atomData[i]), &(dest->atomData[i]));
00602     }
00603     Vmem_free(thee->vmem, thee->nAtomData, sizeof(Vparam_AtomData),
00604       (void **)&(thee->atomData));
00605 }
00606
00607 VEXTERNC void Vparam_AtomData_copyFrom(Vparam_AtomData *thee,
00608   Vparam_AtomData *src) { Vparam_AtomData_copyTo(src, thee); }
00609
00610 VPRIVATE int readXMLFileAtom(Vio *sock, Vparam_AtomData *atom) {
00611
00612     double dtmp;
00613     char tok[VMAX_BUFSIZE];
00614     int chgflag, radflag, nameflag;
00615
00616     VASSERT(atom != VNULL);
00617
00618     if (Vio_scanf(sock, "%s", tok) != 1) return 0;
00619
00620     chgflag = 0;
00621     radflag = 0;
00622     nameflag = 0;
00623
00624     while (1)
00625     {
00626         if (Vstring_strcasecmp(tok, "name") == 0) {
00627             VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00628             if (strlen(tok) > VMAX_ARGLEN) {
00629                 Vnm_print(2, "Vparam_readXMLFileAtom: string (%s) too long \
00630 (%d)!\n", tok, strlen(tok));
00631                 return 0;
00632             }
00633             nameflag = 1;
00634             strcpy(atom->atomName, tok);
00635         } else if (Vstring_strcasecmp(tok, "charge") == 0) {
00636             VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00637             if (sscanf(tok, "%lf", &dtmp) != 1) {
00638                 Vnm_print(2, "Vparam_readXMLFileAtom: Unexpected token (%s) while \
00639 parsing charge!\n", tok);
00640                 return 0;
00641             }
00642             chgflag = 1;
00643             atom->charge = dtmp;
00644         } else if (Vstring_strcasecmp(tok, "radius") == 0) {
00645             VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00646             if (sscanf(tok, "%lf", &dtmp) != 1) {
00647                 Vnm_print(2, "Vparam_readXMLFileAtom: Unexpected token (%s) while \
00648 parsing radius!\n", tok);
00649                 return 0;
00650             }
00651             radflag = 1;
00652             atom->radius = dtmp;
00653         } else if (Vstring_strcasecmp(tok, "epsilon") == 0) {
00654             VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00655             if (sscanf(tok, "%lf", &dtmp) != 1) {
00656                 Vnm_print(2, "Vparam_readXMLFileAtom: Unexpected token (%s) while \
00657 parsing epsilon!\n", tok);
00658                 return 0;
00659             }
00660             atom->epsilon = dtmp;
00661         } else if ((Vstring_strcasecmp(tok, "/atom") == 0) ||
00662             (Vstring_strcasecmp(tok, "atom") == 0)){
00663             if (chgflag && radflag && nameflag) return 1;
00664             else if (!chgflag) {

```

```

00665             Vnm_print(2, "Vparam_readXMLFileAtom: Reached end of atom without \
00666 setting the charge!\n");
00667             return 0;
00668         } else if (!radflag) {
00669             Vnm_print(2, "Vparam_readXMLFileAtom: Reached end of atom without \
00670 setting the radius!\n");
00671             return 0;
00672         } else if (!nameflag) {
00673             Vnm_print(2, "Vparam_readXMLFileAtom: Reached end of atom without \
00674 setting the name!\n");
00675             return 0;
00676         }
00677     }
00678     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00679 }
00680
00681 /* If we get here something wrong has happened */
00682
00683 VJMPERR1(1);
00684
00685 ERROR1:
00686     Vnm_print(2, "Vparam_readXMLFileAtom: Got unexpected EOF reading parameter file!\n");
00687     return 0;
00688 }
00689
00690
00691 VPRIVATE int readFlatFileLine(Vio *sock, Vparam_AtomData *atom) {
00692     double dtmp;
00693     char tok[VMAX_BUFSIZE];
00694
00695     VASSERT(atom != VNULL);
00696
00697     if (Vio_scanf(sock, "%s", tok) != 1) return 0;
00698     if (strlen(tok) > VMAX_ARGLEN) {
00699         Vnm_print(2, "Vparam_readFlatFile: string (%s) too long (%d)!\n",
00700 tok, strlen(tok));
00701         return 0;
00702     }
00703     strcpy(atom->resName, tok);
00704     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00705     if (strlen(tok) > VMAX_ARGLEN) {
00706         Vnm_print(2, "Vparam_readFlatFile: string (%s) too long (%d)!\n",
00707 tok, strlen(tok));
00708         return 0;
00709     }
00710     strcpy(atom->atomName, tok);
00711     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00712     if (sscanf(tok, "%lf", &dtmp) != 1) {
00713         Vnm_print(2, "Vparam_readFlatFile: Unexpected token (%s) while \
00714 parsing charge!\n", tok);
00715         return 0;
00716     }
00717     atom->charge = dtmp;
00718     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00719     if (sscanf(tok, "%lf", &dtmp) != 1) {
00720         Vnm_print(2, "Vparam_readFlatFile: Unexpected token (%s) while \
00721 parsing radius!\n", tok);
00722         return 0;
00723     }
00724     atom->radius = dtmp;
00725     VJMPERR1(Vio_scanf(sock, "%s", tok) == 1);
00726     if (sscanf(tok, "%lf", &dtmp) != 1) {
00727         Vnm_print(2, "Vparam_readFlatFile: Unexpected token (%s) while \
00728 parsing radius!\n", tok);
00729         return 0;
00730     }
00731     atom->epsilon = dtmp;
00732     return 1;
00733 }
00734
00735 ERROR1:
00736     Vnm_print(2, "Vparam_readFlatFile: Got unexpected EOF reading parameter file!\n");
00737     return 0;
00738 }
00739

```


- struct [Vparam](#)
Reads and assigns charge/radii parameters.

Typedefs

- typedef struct [sVparam_AtomData](#) [Vparam_AtomData](#)
Declaration of the Vparam_AtomData class as the sVparam_AtomData structure.
- typedef struct [Vparam_ResData](#) [Vparam_ResData](#)
- typedef struct [Vparam](#) [Vparam](#)

Functions

- VEXTERNC unsigned long int [Vparam_memChk](#) ([Vparam](#) *thee)
Get number of bytes in this object and its members.
- VEXTERNC [Vparam_AtomData](#) * [Vparam_AtomData_ctor](#) ()
Construct the object.
- VEXTERNC int [Vparam_AtomData_ctor2](#) ([Vparam_AtomData](#) *thee)
FORTTRAN stub to construct the object.
- VEXTERNC void [Vparam_AtomData_dtor](#) ([Vparam_AtomData](#) **thee)
Destroy object.
- VEXTERNC void [Vparam_AtomData_dtor2](#) ([Vparam_AtomData](#) *thee)
FORTTRAN stub to destroy object.
- VEXTERNC void [Vparam_AtomData_copyTo](#) ([Vparam_AtomData](#) *thee, [Vparam_AtomData](#) *dest)
Copy current atom object to destination.
- VEXTERNC void [Vparam_ResData_copyTo](#) ([Vparam_ResData](#) *thee, [Vparam_ResData](#) *dest)
Copy current residue object to destination.
- VEXTERNC void [Vparam_AtomData_copyFrom](#) ([Vparam_AtomData](#) *thee, [Vparam_AtomData](#) *src)
Copy current atom object from another.
- VEXTERNC [Vparam_ResData](#) * [Vparam_ResData_ctor](#) (Vmem *mem)
Construct the object.
- VEXTERNC int [Vparam_ResData_ctor2](#) ([Vparam_ResData](#) *thee, Vmem *mem)
FORTTRAN stub to construct the object.
- VEXTERNC void [Vparam_ResData_dtor](#) ([Vparam_ResData](#) **thee)
Destroy object.
- VEXTERNC void [Vparam_ResData_dtor2](#) ([Vparam_ResData](#) *thee)
FORTTRAN stub to destroy object.
- VEXTERNC [Vparam](#) * [Vparam_ctor](#) ()
Construct the object.
- VEXTERNC int [Vparam_ctor2](#) ([Vparam](#) *thee)
FORTTRAN stub to construct the object.
- VEXTERNC void [Vparam_dtor](#) ([Vparam](#) **thee)
Destroy object.
- VEXTERNC void [Vparam_dtor2](#) ([Vparam](#) *thee)
FORTTRAN stub to destroy object.
- VEXTERNC [Vparam_ResData](#) * [Vparam_getResData](#) ([Vparam](#) *thee, char resName[VMAX_ARGLEN])
Get residue data.
- VEXTERNC [Vparam_AtomData](#) * [Vparam_getAtomData](#) ([Vparam](#) *thee, char resName[VMAX_ARGLEN], char atomName[VMAX_ARGLEN])

Get atom data.

- VEXTERNC int [Vparam_readFlatFile](#) ([Vparam](#) *thee, const char *iodev, const char *iofmt, const char *thost, const char *fname)

Read a flat-file format parameter database.

- VEXTERNC int [Vparam_readXMLFile](#) ([Vparam](#) *thee, const char *iodev, const char *iofmt, const char *thost, const char *fname)

Read an XML format parameter database.

9.80.1 Detailed Description

Contains declarations for class [Vparam](#).

Version

\$Id\$

Author

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Attention

```
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```

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* THE POSSIBILITY OF SUCH DAMAGE.
*
*
```

Definition in file [vparam.h](#).

9.80.2 Typedef Documentation

9.80.2.1 Vparam

typedef struct [Vparam](#) [Vparam](#)

Definition at line 147 of file [vparam.h](#).

9.80.2.2 Vparam_ResData

typedef struct [Vparam_ResData](#) [Vparam_ResData](#)

Definition at line 127 of file [vparam.h](#).

9.81 vparam.h

[Go to the documentation of this file.](#)

```

00001
00062 #ifndef _VPARAM_H_
00063 #define _VPARAM_H_
00064
00065 #include "apbscfg.h"
00066
00067 #include "malloc/malloc.h"
00068 #if defined(HAVE_MC_H)
00069 #include "mc/mc.h"
00070 #endif
00071
00072 #include "generic/vhal.h"
00073 #include "generic/vunit.h"
00074 #include "generic/vstring.h"
00075
00092 struct sVparam_AtomData {
00093     char atomName[VMAX_ARGLEN];
00094     char resName[VMAX_ARGLEN];
00095     double charge;
00096     double radius;
00097     double epsilon;
00099 };
00100
00106 typedef struct sVparam_AtomData Vparam_AtomData;
00107
00114 struct Vparam_ResData {
00115     Vmem *vmem;
00116     char name[VMAX_ARGLEN];
00117     int nAtomData;
00119     Vparam_AtomData *atomData;
00120 };
00121
00127 typedef struct Vparam_ResData Vparam_ResData;
00128
00135 struct Vparam {
00136
00137     Vmem *vmem;
00138     int nResData;
00140     Vparam_ResData *resData;
00141 };
00142
00147 typedef struct Vparam Vparam;
00148
00149 /* ////////////////////////////////////// */
00150 // Class Vparam: Inlineable methods (vparam.c)
00152
00153 #if !defined(VINLINE_VPARAM)
00154
00161     VEXTERNC unsigned long int Vparam_memChk(Vparam *thee);
```

```

00162
00163 #else /* if defined(VINLINE_VPARAM) */
00164
00165 #   define Vparam_memChk(thee) (Vmem_bytes((thee)->vmem))
00166
00167 #endif /* if !defined(VINLINE_VPARAM) */
00168
00169 /* ////////////////////////////////////// */
00170 // Class Vparam: Non-Inlineable methods (vparam.c)
00171
00172
00173 VEXTERNC Vparam_AtomData* Vparam_AtomData_ctor();
00174
00175 VEXTERNC int Vparam_AtomData_ctor2(Vparam_AtomData *thee);
00176
00177 VEXTERNC void Vparam_AtomData_dtor(Vparam_AtomData **thee);
00178
00179 VEXTERNC void Vparam_AtomData_dtor2(Vparam_AtomData *thee);
00180
00181 VEXTERNC void Vparam_AtomData_copyTo(Vparam_AtomData *thee,
00182   Vparam_AtomData *dest);
00183
00184 VEXTERNC void Vparam_ResData_copyTo(Vparam_ResData *thee,
00185   Vparam_ResData *dest);
00186
00187 VEXTERNC void Vparam_AtomData_copyFrom(Vparam_AtomData *thee,
00188   Vparam_AtomData *src);
00189
00190 VEXTERNC Vparam_ResData* Vparam_ResData_ctor(Vmem *mem);
00191
00192 VEXTERNC int Vparam_ResData_ctor2(Vparam_ResData *thee, Vmem *mem);
00193
00194 VEXTERNC void Vparam_ResData_dtor(Vparam_ResData **thee);
00195
00196 VEXTERNC void Vparam_ResData_dtor2(Vparam_ResData *thee);
00197
00198 VEXTERNC Vparam* Vparam_ctor();
00199
00200 VEXTERNC int Vparam_ctor2(Vparam *thee);
00201
00202 VEXTERNC void Vparam_dtor(Vparam **thee);
00203
00204 VEXTERNC void Vparam_dtor2(Vparam *thee);
00205
00206 VEXTERNC Vparam_ResData* Vparam_getResData(Vparam *thee,
00207   char resName[VMAX_ARGLEN]);
00208
00209 VEXTERNC Vparam_AtomData* Vparam_getAtomData(Vparam *thee,
00210   char resName[VMAX_ARGLEN], char atomName[VMAX_ARGLEN]);
00211
00212 VEXTERNC int Vparam_readFlatFile(Vparam *thee, const char *iodev,
00213   const char *iofmt, const char *thost, const char *fname);
00214
00215 VEXTERNC int Vparam_readXMLFile(Vparam *thee, const char *iodev,
00216   const char *iofmt, const char *thost, const char *fname);
00217
00218 #endif /* ifndef _VPARAM_H_ */

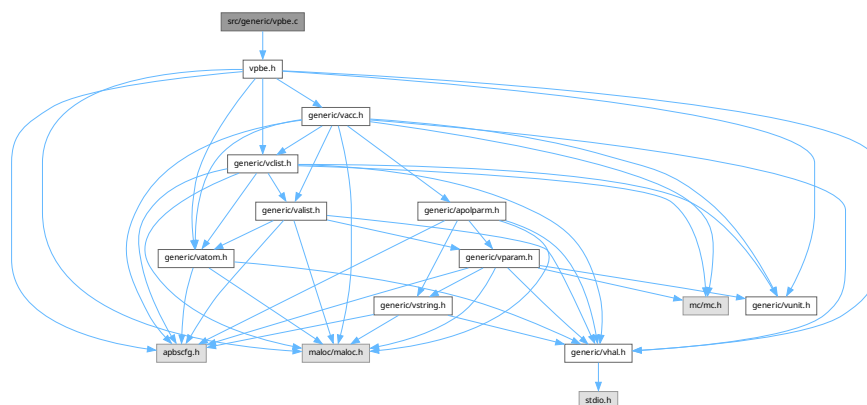
```

9.82 src/generic/vpbe.c File Reference

Class Vpbe methods.

```
#include "vpbe.h"
```

Include dependency graph for vpbe.c:



Macros

- #define `MAX_SPLINE_WINDOW` 0.5

Functions

- VPUBLIC `Valist *` `Vpbe_getValist` (`Vpbe *``thee`)
Get atom list.
- VPUBLIC `Vacc *` `Vpbe_getVacc` (`Vpbe *``thee`)
Get accessibility oracle.
- VPUBLIC double `Vpbe_getBulkIonicStrength` (`Vpbe *``thee`)
Get bulk ionic strength.
- VPUBLIC double `Vpbe_getTemperature` (`Vpbe *``thee`)
Get temperature.
- VPUBLIC double `Vpbe_getSoluteDiel` (`Vpbe *``thee`)
Get solute dielectric constant.
- VPUBLIC double * `Vpbe_getSoluteCenter` (`Vpbe *``thee`)
Get coordinates of solute center.
- VPUBLIC double `Vpbe_getSolventDiel` (`Vpbe *``thee`)
Get solvent dielectric constant.
- VPUBLIC double `Vpbe_getSolventRadius` (`Vpbe *``thee`)
Get solvent molecule radius.
- VPUBLIC double `Vpbe_getMaxIonRadius` (`Vpbe *``thee`)
Get maximum radius of ion species.
- VPUBLIC double `Vpbe_getXkappa` (`Vpbe *``thee`)
Get Debye-Huckel parameter.
- VPUBLIC double `Vpbe_getDeblen` (`Vpbe *``thee`)
Get Debye-Huckel screening length.
- VPUBLIC double `Vpbe_getZkappa2` (`Vpbe *``thee`)
Get modified squared Debye-Huckel parameter.
- VPUBLIC double `Vpbe_getZmagic` (`Vpbe *``thee`)

- Get charge scaling factor.*

 - VPUBLIC double [Vpbe_getSoluteRadius](#) ([Vpbe](#) *thee)
- Get sphere radius which bounds biomolecule.*

 - VPUBLIC double [Vpbe_getSoluteXlen](#) ([Vpbe](#) *thee)
- Get length of solute in x dimension.*

 - VPUBLIC double [Vpbe_getSoluteYlen](#) ([Vpbe](#) *thee)
- Get length of solute in y dimension.*

 - VPUBLIC double [Vpbe_getSoluteZlen](#) ([Vpbe](#) *thee)
- Get length of solute in z dimension.*

 - VPUBLIC double [Vpbe_getSoluteCharge](#) ([Vpbe](#) *thee)
- Get total solute charge.*

 - VPUBLIC double [Vpbe_getzmem](#) ([Vpbe](#) *thee)
- Get z position of the membrane bottom.*

 - VPUBLIC double [Vpbe_getLmem](#) ([Vpbe](#) *thee)
- Get length of the membrane (A)*
aaauthor Michael Grabe.

 - VPUBLIC double [Vpbe_getmembraneDiel](#) ([Vpbe](#) *thee)
- Get membrane dielectric constant.*

 - VPUBLIC double [Vpbe_getmemv](#) ([Vpbe](#) *thee)
- Get membrane potential (kT)*

 - VPUBLIC [Vpbe](#) * [Vpbe_ctor](#) ([Valist](#) *alist, int ionNum, double *ionConc, double *ionRadii, double *ionQ, double T, double soluteDiel, double solventDiel, double solventRadius, int focusFlag, double sdens, double z_mem, double L, double membraneDiel, double V)
- Construct Vpbe object.*

 - VPUBLIC int [Vpbe_ctor2](#) ([Vpbe](#) *thee, [Valist](#) *alist, int ionNum, double *ionConc, double *ionRadii, double *ionQ, double T, double soluteDiel, double solventDiel, double solventRadius, int focusFlag, double sdens, double z_mem, double L, double membraneDiel, double V)
- FORTTRAN stub to construct Vpbe object.*

 - VPUBLIC void [Vpbe_dtor](#) ([Vpbe](#) **thee)
- Object destructor.*

 - VPUBLIC void [Vpbe_dtor2](#) ([Vpbe](#) *thee)
- FORTTRAN stub object destructor.*

 - VPUBLIC double [Vpbe_getCoulombEnergy1](#) ([Vpbe](#) *thee)
- Calculate coulombic energy of set of charges.*

 - VPUBLIC unsigned long int [Vpbe_memChk](#) ([Vpbe](#) *thee)
- Return the memory used by this structure (and its contents) in bytes.*

 - VPUBLIC int [Vpbe_getIons](#) ([Vpbe](#) *thee, int *nion, double ionConc[[MAXION](#)], double ionRadii[[MAXION](#)], double ionQ[[MAXION](#)])
- Get information about the counterion species present.*

9.82.1 Detailed Description

Class Vpbe methods.

Author

Nathan Baker

Version

\$Id\$

Attention

```
*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
*   Nathan A. Baker (nathan.baker@pnnl.gov)
*   Pacific Northwest National Laboratory
*
*   Additional contributing authors listed in the code documentation.
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*
*
```

Definition in file [vpbe.c](#).

9.82.2 Macro Definition Documentation

9.82.2.1 MAX_SPLINE_WINDOW

```
#define MAX_SPLINE_WINDOW 0.5
```

Definition at line 62 of file [vpbe.c](#).

9.83 vpbe.c

[Go to the documentation of this file.](#)

```
00001
00057 #include "vpbe.h"
00058
00059 /* ////////////////////////////////////////
00060 // Class Vpbe: Private method declaration
00062 #define MAX_SPLINE_WINDOW 0.5
00063
00064 /* ////////////////////////////////////////
00065 // Class Vpbe: Inlineable methods
00067 #if !defined(VINLINE_VPBE)
00068
00069 VPUBLIC Valist* Vpbe_getValist(Vpbe *thee) {
00070
00071     VASSERT(thee != VNULL);
00072     return thee->alist;
00073 }
00074 }
00075
00076 VPUBLIC Vacc* Vpbe_getVacc(Vpbe *thee) {
00077
00078     VASSERT(thee != VNULL);
00079     VASSERT(thee->paramFlag);
00080     return thee->acc;
00081 }
00082 }
00083
00084 VPUBLIC double Vpbe_getBulkIonicStrength(Vpbe *thee) {
00085
00086     VASSERT(thee != VNULL);
00087     VASSERT(thee->paramFlag);
00088     return thee->bulkIonicStrength;
00089 }
00090
00091 VPUBLIC double Vpbe_getTemperature(Vpbe *thee) {
00092
00093     VASSERT(thee != VNULL);
00094     VASSERT(thee->paramFlag);
00095     return thee->T;
00096 }
00097 }
00098
00099 VPUBLIC double Vpbe_getSoluteDiel(Vpbe *thee) {
00100
00101     VASSERT(thee != VNULL);
00102     VASSERT(thee->paramFlag);
00103     return thee->soluteDiel;
00104 }
00105 }
00106
00107 VPUBLIC double* Vpbe_getSoluteCenter(Vpbe *thee) {
00108
00109     VASSERT(thee != VNULL);
00110     return thee->soluteCenter;
00111 }
00112
00113 VPUBLIC double Vpbe_getSolventDiel(Vpbe *thee) {
00114
00115     VASSERT(thee != VNULL);
00116     VASSERT(thee->paramFlag);
00117     return thee->solventDiel;
00118 }
00119
00120 VPUBLIC double Vpbe_getSolventRadius(Vpbe *thee) {
00121
00122     VASSERT(thee != VNULL);
00123     VASSERT(thee->paramFlag);
00124     return thee->solventRadius;
00125 }
00126
00127 VPUBLIC double Vpbe_getMaxIonRadius(Vpbe *thee) {
00128
00129     VASSERT(thee != VNULL);
00130     VASSERT(thee->paramFlag);
00131     return thee->maxIonRadius;
00132 }
00133
00134 VPUBLIC double Vpbe_getXkappa(Vpbe *thee) {
00135
00136     VASSERT(thee != VNULL);
00137     VASSERT(thee->paramFlag);
00138     return thee->xkappa;
```



```

00139 }
00140
00141 VPUBLIC double Vpbe_getDeblen(Vpbe *thee) {
00142     VASSERT(thee != VNULL);
00143     VASSERT(thee->paramFlag);
00144     return thee->deblen;
00145 }
00146
00147
00148 VPUBLIC double Vpbe_getZkappa2(Vpbe *thee) {
00149     VASSERT(thee != VNULL);
00150     VASSERT(thee->paramFlag);
00151     return thee->zkappa2;
00152 }
00153
00154
00155 VPUBLIC double Vpbe_getZmagic(Vpbe *thee) {
00156     VASSERT(thee != VNULL);
00157     VASSERT(thee->paramFlag);
00158     return thee->zmagic;
00159 }
00160
00161
00162 VPUBLIC double Vpbe_getSoluteRadius(Vpbe *thee) {
00163     VASSERT(thee != VNULL);
00164     return thee->soluteRadius;
00165 }
00166
00167
00168 VPUBLIC double Vpbe_getSoluteXlen(Vpbe *thee) {
00169     VASSERT(thee != VNULL);
00170     return thee->soluteXlen;
00171 }
00172
00173
00174 VPUBLIC double Vpbe_getSoluteYlen(Vpbe *thee) {
00175     VASSERT(thee != VNULL);
00176     return thee->soluteYlen;
00177 }
00178
00179
00180 VPUBLIC double Vpbe_getSoluteZlen(Vpbe *thee) {
00181     VASSERT(thee != VNULL);
00182     return thee->soluteZlen;
00183 }
00184
00185
00186 VPUBLIC double Vpbe_getSoluteCharge(Vpbe *thee) {
00187     VASSERT(thee != VNULL);
00188     return thee->soluteCharge;
00189 }
00190
00191
00192 /* ////////////////////////////////////////
00193 // Routine: Vpbe_getzmem
00194 // Purpose: This routine returns values stored in the structure thee.
00195 // Author: Michael Grabe
00197 VPUBLIC double Vpbe_getzmem(Vpbe *thee) {
00198     VASSERT(thee != VNULL);
00199     VASSERT(thee->param2Flag);
00200     return thee->z_mem;
00201 }
00202
00203
00204 /* ////////////////////////////////////////
00205 // Routine: Vpbe_getLmem
00206 // Purpose: This routine returns values stored in the structure thee.
00207 // Author: Michael Grabe
00209 VPUBLIC double Vpbe_getLmem(Vpbe *thee) {
00210     VASSERT(thee != VNULL);
00211     VASSERT(thee->param2Flag);
00212     return thee->L;
00213 }
00214
00215
00216 /* ////////////////////////////////////////
00217 // Routine: Vpbe_getmembraneDiel
00218 // Purpose: This routine returns values stored in the structure thee.
00219 // Author: Michael Grabe
00221 VPUBLIC double Vpbe_getmembraneDiel(Vpbe *thee) {
00222

```

```

00223     VASSERT(thee != VNULL);
00224     VASSERT(thee->param2Flag);
00225     return thee->membraneDiel;
00226 }
00227
00228 /* ////////////////////////////////////// */
00229 // Routine: Vpbe_getmemv
00230 // Purpose: This routine returns values stored in the structure thee.
00231 // Author: Michael Grabe
00233 VPUBLIC double Vpbe_getmemv(Vpbe *thee) {
00234
00235     VASSERT(thee != VNULL);
00236     VASSERT(thee->param2Flag);
00237     return thee->V;
00238 }
00239
00240 #endif /* if !defined(VINLINE_VPBE) */
00241
00242 /* ////////////////////////////////////// */
00243 // Class Vpbe: Non-inlineable methods
00244
00246 VPUBLIC Vpbe* Vpbe_ctor(Valist *alist, int ionNum, double *ionConc,
00247                        double *ionRadii, double *ionQ, double T,
00248                        double soluteDiel, double solventDiel,
00249                        double solventRadius, int focusFlag, double sdens,
00250                        double z_mem, double L, double membraneDiel, double V ) {
00251
00252     /* Set up the structure */
00253     Vpbe *thee = VNULL;
00254     thee = (Vpbe*)Vmem_malloc(VNULL, 1, sizeof(Vpbe) );
00255     VASSERT( thee != VNULL);
00256     VASSERT( Vpbe_ctor2(thee, alist, ionNum, ionConc, ionRadii, ionQ,
00257                        T, soluteDiel, solventDiel, solventRadius, focusFlag, sdens,
00258                        z_mem, L, membraneDiel, V) );
00259
00260     return thee;
00261 }
00262
00263
00264 VPUBLIC int Vpbe_ctor2(Vpbe *thee, Valist *alist, int ionNum,
00265                      double *ionConc, double *ionRadii,
00266                      double *ionQ, double T, double soluteDiel,
00267                      double solventDiel, double solventRadius, int focusFlag,
00268                      double sdens, double z_mem, double L, double membraneDiel,
00269                      double V) {
00270
00271     int i, iatom, inhash[3];
00272     double atomRadius;
00273     Vatom *atom;
00274     double center[3] = {0.0, 0.0, 0.0};
00275     double lower_corner[3] = {0.0, 0.0, 0.0};
00276     double upper_corner[3] = {0.0, 0.0, 0.0};
00277     double disp[3], dist, radius, charge, xmin, xmax, ymin, ymax, zmin, zmax;
00278     double x, y, z, netCharge;
00279     double nhash[3];
00280     const double N_A = 6.022045000e+23;
00281     const double e_c = 4.803242384e-10;
00282     const double k_B = 1.380662000e-16;
00283     const double pi = 4. * VATAN(1.);
00284
00285     /* Set up memory management object */
00286     thee->vmem = Vmem_ctor("APBS:VPBE");
00287
00288     VASSERT(thee != VNULL);
00289     if (alist == VNULL) {
00290         Vnm_print(2, "Vpbe_ctor2: Got null pointer to Valist object!\n");
00291         return 0;
00292     }
00293
00294     /* **** STUFF THAT GETS DONE FOR EVERYONE **** */
00295     /* Set pointers */
00296     thee->alist = alist;
00297     thee->paramFlag = 0;
00298
00299     /* Determine solute center */
00300     center[0] = thee->alist->center[0];
00301     center[1] = thee->alist->center[1];
00302     center[2] = thee->alist->center[2];
00303     thee->soluteCenter[0] = center[0];
00304     thee->soluteCenter[1] = center[1];
00305     thee->soluteCenter[2] = center[2];

```

```

00306
00307  /* Determine solute length and charge */
00308  radius = 0;
00309  atom = Valist_getAtom(thee->alist, 0);
00310  xmin = Vatom_getPosition(atom)[0];
00311  xmax = Vatom_getPosition(atom)[0];
00312  ymin = Vatom_getPosition(atom)[1];
00313  ymax = Vatom_getPosition(atom)[1];
00314  zmin = Vatom_getPosition(atom)[2];
00315  zmax = Vatom_getPosition(atom)[2];
00316  charge = 0;
00317  for (iatom=0; iatom<Valist_getNumberAtoms(thee->alist); iatom++) {
00318      atom = Valist_getAtom(thee->alist, iatom);
00319      atomRadius = Vatom_getRadius(atom);
00320      x = Vatom_getPosition(atom)[0];
00321      y = Vatom_getPosition(atom)[1];
00322      z = Vatom_getPosition(atom)[2];
00323      if ((x+atomRadius) > xmax) xmax = x + atomRadius;
00324      if ((x-atomRadius) < xmin) xmin = x - atomRadius;
00325      if ((y+atomRadius) > ymax) ymax = y + atomRadius;
00326      if ((y-atomRadius) < ymin) ymin = y - atomRadius;
00327      if ((z+atomRadius) > zmax) zmax = z + atomRadius;
00328      if ((z-atomRadius) < zmin) zmin = z - atomRadius;
00329      disp[0] = (x - center[0]);
00330      disp[1] = (y - center[1]);
00331      disp[2] = (z - center[2]);
00332      dist = (disp[0]*disp[0] + (disp[1]*disp[1] + (disp[2]*disp[2]));
00333      dist = VSQRT(dist) + atomRadius;
00334      if (dist > radius) radius = dist;
00335      charge += Vatom_getCharge(Valist_getAtom(thee->alist, iatom));
00336  }
00337  thee->soluteRadius = radius;
00338  Vnm_print(0, "Vpbe_ctor2: solute radius = %g\n", radius);
00339  thee->soluteXlen = xmax - xmin;
00340  thee->soluteYlen = ymax - ymin;
00341  thee->soluteZlen = zmax - zmin;
00342  Vnm_print(0, "Vpbe_ctor2: solute dimensions = %g x %g x %g\n",
00343      thee->soluteXlen, thee->soluteYlen, thee->soluteZlen);
00344  thee->soluteCharge = charge;
00345  Vnm_print(0, "Vpbe_ctor2: solute charge = %g\n", charge);
00346
00347  /* Set parameters */
00348  thee->numIon = ionNum;
00349  if (thee->numIon >= MAXION) {
00350      Vnm_print(2, "Vpbe_ctor2: Too many ion species (MAX = %d)!\n",
00351          MAXION);
00352      return 0;
00353  }
00354  thee->bulkIonicStrength = 0.0;
00355  thee->maxIonRadius = 0.0;
00356  netCharge = 0.0;
00357  for (i=0; i<thee->numIon; i++) {
00358      thee->ionConc[i] = ionConc[i];
00359      thee->ionRadii[i] = ionRadii[i];
00360      if (ionRadii[i] > thee->maxIonRadius) thee->maxIonRadius = ionRadii[i];
00361      thee->ionQ[i] = ionQ[i];
00362      thee->bulkIonicStrength += (0.5*ionConc[i]*VSQR(ionQ[i]));
00363      netCharge += (ionConc[i]*ionQ[i]);
00364  }
00365  #ifndef VAPBSQUIET
00366      Vnm_print(1, " Vpbe_ctor: Using max ion radius (%g A) for exclusion \
00367  function\n", thee->maxIonRadius);
00368  #endif
00369  if (VABS(netCharge) > VSMALL) {
00370      Vnm_print(2, "Vpbe_ctor2: You have a counterion charge imbalance!\n");
00371      Vnm_print(2, "Vpbe_ctor2: Net charge conc. = %g M\n", netCharge);
00372      return 0;
00373  }
00374  thee->T = T;
00375  thee->soluteDiel = soluteDiel;
00376  thee->solventDiel = solventDiel;
00377  thee->solventRadius = solventRadius;
00378
00379  /* Compute parameters:
00380  *
00381  *  $\kappa^2 = (8 \pi N_A e_c^2) I_s / (1000 \epsilon_w k_B T)$ 
00382  *  $\kappa = 0.325567 * I_s^{1/2}$  angstroms-1
00383  *  $deblen = 1 / \kappa$ 
00384  *  $= 3.071564378 * I_s^{1/2}$  angstroms
00385  *  $\bar{\kappa}^2 = \epsilon_w * \kappa^2$ 
00386  *  $zmagic = (4 * \pi * e_c^2) / (k_B T)$  (we scale the diagonal later)

```

```

00387      *          = 7046.528838
00388      */
00389      if (thee->T == 0.0) {
00390          Vnm_print(2, "Vpbe_ctor2: You set the temperature to 0 K.\n");
00391          Vnm_print(2, "Vpbe_ctor2: That violates the 3rd Law of Thermo!");
00392          return 0;
00393      }
00394      if (thee->bulkIonicStrength == 0.) {
00395          thee->xkappa = 0.;
00396          thee->deblen = 0.;
00397          thee->zkappa2 = 0.;
00398      } else {
00399          thee->xkappa = VSQRT( thee->bulkIonicStrength * 1.0e-16 *
00400              ((8.0 * pi * N_A * e_c*e_c) /
00401              (1000.0 * thee->solventDiel * k_B * T))
00402          );
00403          thee->deblen = 1. / thee->xkappa;
00404          thee->zkappa2 = thee->solventDiel * VSQR(thee->xkappa);
00405      }
00406      Vnm_print(0, "Vpbe_ctor2: bulk ionic strength = %g\n",
00407          thee->bulkIonicStrength);
00408      Vnm_print(0, "Vpbe_ctor2: xkappa = %g\n", thee->xkappa);
00409      Vnm_print(0, "Vpbe_ctor2: Debye length = %g\n", thee->deblen);
00410      Vnm_print(0, "Vpbe_ctor2: zkappa2 = %g\n", thee->zkappa2);
00411      thee->zmagic = ((4.0 * pi * e_c*e_c) / (k_B * thee->T)) * 1.0e+8;
00412      Vnm_print(0, "Vpbe_ctor2: zmagic = %g\n", thee->zmagic);
00413
00414      /* Compute accessibility objects:
00415      *   - Allow for extra room in the case of spline windowing
00416      *   - Place some limits on the size of the hash table in the case of very
00417      *       large molecules
00418      */
00419      if (thee->maxIonRadius > thee->solventRadius)
00420          radius = thee->maxIonRadius + MAX_SPLINE_WINDOW;
00421      else radius = thee->solventRadius + MAX_SPLINE_WINDOW;
00422
00423      nhash[0] = (thee->soluteXlen)/0.5;
00424      nhash[1] = (thee->soluteYlen)/0.5;
00425      nhash[2] = (thee->soluteZlen)/0.5;
00426      for (i=0; i<3; i++) inhash[i] = (int) (nhash[i]);
00427
00428      for (i=0; i<3; i++){
00429          if (inhash[i] < 3) inhash[i] = 3;
00430          if (inhash[i] > MAX_HASH_DIM) inhash[i] = MAX_HASH_DIM;
00431      }
00432      Vnm_print(0, "Vpbe_ctor2: Constructing Vclist with %d x %d x %d table\n",
00433          inhash[0], inhash[1], inhash[2]);
00434
00435      thee->clist = Vclist_ctor(thee->alist, radius, inhash,
00436          CLIST_AUTO_DOMAIN, lower_corner, upper_corner);
00437
00438      VASSERT(thee->clist != VNULL);
00439      thee->acc = Vacc_ctor(thee->alist, thee->clist, sdens);
00440
00441      VASSERT(thee->acc != VNULL);
00442
00443      /* SMPBE Added */
00444      thee->smsize = 0.0;
00445      thee->smvolume = 0.0;
00446      thee->ipkey = 0;
00447
00448      thee->paramFlag = 1;
00449
00450      /*-----*/
00451      /* added by Michael Grabe */
00452      /*-----*/
00453
00454      thee->z_mem = z_mem;
00455      thee->L = L;
00456      thee->membraneDiel = membraneDiel;
00457      thee->V = V;
00458
00459      if (V != 0.0) thee->param2Flag = 1;
00460      else thee->param2Flag = 0;
00461
00462      /*-----*/
00463
00464      return 1;
00465 }
00466
00467 VPUBLIC void Vpbe_dtor(Vpbe **thee) {

```

```

00468     if ((*thee) != VNULL) {
00469         Vpbe_dtor2(*thee);
00470         Vmem_free(VNULL, 1, sizeof(Vpbe), (void **)thee);
00471         (*thee) = VNULL;
00472     }
00473 }
00474
00475 VPUBLIC void Vpbe_dtor2(Vpbe *thee) {
00476     Vclist_dtor(&(thee->clist));
00477     Vacc_dtor(&(thee->acc));
00478     Vmem_dtor(&(thee->vmem));
00479 }
00480
00481 VPUBLIC double Vpbe_getCoulombEnergy1(Vpbe *thee) {
00482     int i, j, k, natoms;
00483     double dist, *ipos, *jpos, icharge, jcharge;
00484     double energy = 0.0;
00485     double eps, T;
00486     Vatom *iatom, *jatom;
00487     Valist *alist;
00488     VASSERT(thee != VNULL);
00489     alist = Vpbe_getValist(thee);
00490     VASSERT(alist != VNULL);
00491     natoms = Valist_getNumberAtoms(alist);
00492     /* Do the sum */
00493     for (i=0; i<natoms; i++) {
00494         iatom = Valist_getAtom(alist,i);
00495         icharge = Vatom_getCharge(iatom);
00496         ipos = Vatom_getPosition(iatom);
00497         for (j=i+1; j<natoms; j++) {
00498             jatom = Valist_getAtom(alist,j);
00499             jcharge = Vatom_getCharge(jatom);
00500             jpos = Vatom_getPosition(jatom);
00501             dist = 0;
00502             for (k=0; k<3; k++) dist += ((ipos[k]-jpos[k])*(ipos[k]-jpos[k]));
00503             dist = VSQRT(dist);
00504             energy = energy + icharge*jcharge/dist;
00505         }
00506     }
00507     /* Convert the result to J */
00508     T = Vpbe_getTemperature(thee);
00509     eps = Vpbe_getSoluteDiel(thee);
00510     energy = energy*Vunit_ec*Vunit_ec/(4*Vunit_pi*Vunit_eps0*eps*(1.0e-10));
00511     /* Scale by Boltzmann energy */
00512     energy = energy/(Vunit_kb*T);
00513     return energy;
00514 }
00515
00516 VPUBLIC unsigned long int Vpbe_memChk(Vpbe *thee) {
00517     unsigned long int memUse = 0;
00518     if (thee == VNULL) return 0;
00519     memUse = memUse + sizeof(Vpbe);
00520     memUse = memUse + (unsigned long int)Vacc_memChk(thee->acc);
00521     return memUse;
00522 }
00523
00524 VPUBLIC int Vpbe_getIons(Vpbe *thee, int *nion, double ionConc[MAXION],
00525     double ionRadii[MAXION], double ionQ[MAXION]) {
00526     int i;
00527     VASSERT(thee != VNULL);
00528     *nion = thee->numIon;
00529     for (i=0; i<(*nion); i++) {
00530         ionConc[i] = thee->ionConc[i];
00531         ionRadii[i] = thee->ionRadii[i];
00532         ionQ[i] = thee->ionQ[i];
00533     }
00534 }

```

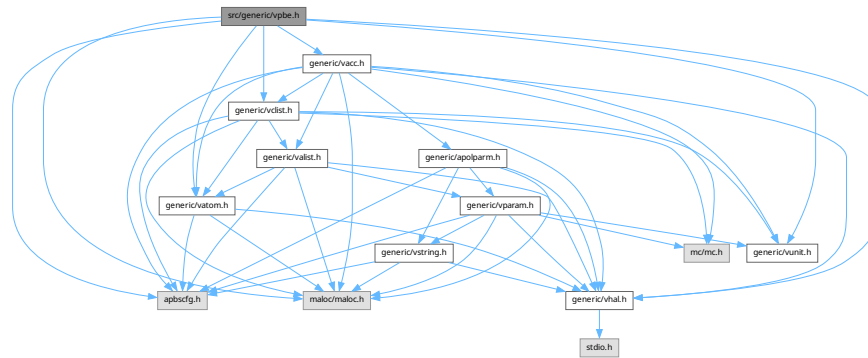
```
00549     return *nion;
00550 }
```

9.84 src/generic/vpbe.h File Reference

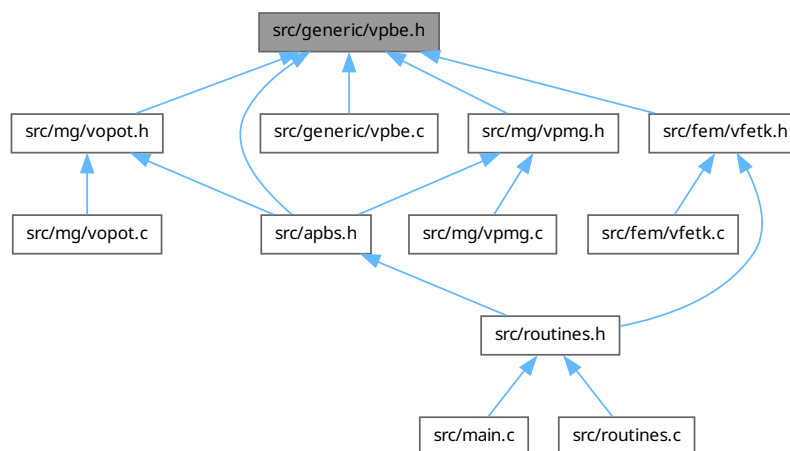
Contains declarations for class Vpbe.

```
#include "apbscfg.h"
#include "malloc/malloc.h"
#include "generic/vhal.h"
#include "generic/vunit.h"
#include "generic/vatom.h"
#include "generic/vacc.h"
#include "generic/vclist.h"
```

Include dependency graph for vpbe.h:



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [sVpbe](#)

Contains public data members for Vpbe class/module.

Typedefs

- typedef struct [sVpbe](#) [Vpbe](#)

Declaration of the Vpbe class as the Vpbe structure.

Functions

- VEXTERNC [Valist](#) * [Vpbe_getValist](#) ([Vpbe](#) *thee)
Get atom list.
- VEXTERNC [Vacc](#) * [Vpbe_getVacc](#) ([Vpbe](#) *thee)
Get accessibility oracle.
- VEXTERNC double [Vpbe_getBulkIonicStrength](#) ([Vpbe](#) *thee)
Get bulk ionic strength.
- VEXTERNC double [Vpbe_getMaxIonRadius](#) ([Vpbe](#) *thee)
Get maximum radius of ion species.
- VEXTERNC double [Vpbe_getTemperature](#) ([Vpbe](#) *thee)
Get temperature.
- VEXTERNC double [Vpbe_getSoluteDiel](#) ([Vpbe](#) *thee)
Get solute dielectric constant.
- VEXTERNC double [Vpbe_getGamma](#) ([Vpbe](#) *thee)
Get apolar coefficient.
- VEXTERNC double [Vpbe_getSoluteRadius](#) ([Vpbe](#) *thee)
Get sphere radius which bounds biomolecule.
- VEXTERNC double [Vpbe_getSoluteXlen](#) ([Vpbe](#) *thee)
Get length of solute in x dimension.
- VEXTERNC double [Vpbe_getSoluteYlen](#) ([Vpbe](#) *thee)
Get length of solute in y dimension.
- VEXTERNC double [Vpbe_getSoluteZlen](#) ([Vpbe](#) *thee)
Get length of solute in z dimension.
- VEXTERNC double * [Vpbe_getSoluteCenter](#) ([Vpbe](#) *thee)
Get coordinates of solute center.
- VEXTERNC double [Vpbe_getSoluteCharge](#) ([Vpbe](#) *thee)
Get total solute charge.
- VEXTERNC double [Vpbe_getSolventDiel](#) ([Vpbe](#) *thee)
Get solvent dielectric constant.
- VEXTERNC double [Vpbe_getSolventRadius](#) ([Vpbe](#) *thee)
Get solvent molecule radius.
- VEXTERNC double [Vpbe_getXkappa](#) ([Vpbe](#) *thee)
Get Debye-Huckel parameter.
- VEXTERNC double [Vpbe_getDeblen](#) ([Vpbe](#) *thee)
Get Debye-Huckel screening length.
- VEXTERNC double [Vpbe_getZkappa2](#) ([Vpbe](#) *thee)
Get modified squared Debye-Huckel parameter.
- VEXTERNC double [Vpbe_getZmagic](#) ([Vpbe](#) *thee)

- Get charge scaling factor.*

 - VEXTERNC double `Vpbe_getzmem` (`Vpbe *thee`)

Get z position of the membrane bottom.
- VEXTERNC double `Vpbe_getLmem` (`Vpbe *thee`)

Get length of the membrane (A)
author Michael Grabe.
- VEXTERNC double `Vpbe_getmembraneDiel` (`Vpbe *thee`)

Get membrane dielectric constant.
- VEXTERNC double `Vpbe_getmemv` (`Vpbe *thee`)

Get membrane potential (kT)
- VEXTERNC `Vpbe * Vpbe_ctor` (`Valist *alist`, `int ionNum`, `double *ionConc`, `double *ionRadii`, `double *ionQ`, `double T`, `double soluteDiel`, `double solventDiel`, `double solventRadius`, `int focusFlag`, `double sdens`, `double z_mem`, `double L`, `double membraneDiel`, `double V`)

Construct Vpbe object.
- VEXTERNC `int Vpbe_ctor2` (`Vpbe *thee`, `Valist *alist`, `int ionNum`, `double *ionConc`, `double *ionRadii`, `double *ionQ`, `double T`, `double soluteDiel`, `double solventDiel`, `double solventRadius`, `int focusFlag`, `double sdens`, `double z_mem`, `double L`, `double membraneDiel`, `double V`)

FORTTRAN stub to construct Vpbe objct.
- VEXTERNC `int Vpbe_getlons` (`Vpbe *thee`, `int *nion`, `double ionConc[MAXION]`, `double ionRadii[MAXION]`, `double ionQ[MAXION]`)

Get information about the counterion species present.
- VEXTERNC `void Vpbe_dtor` (`Vpbe **thee`)

Object destructor.
- VEXTERNC `void Vpbe_dtor2` (`Vpbe *thee`)

FORTTRAN stub object destructor.
- VEXTERNC double `Vpbe_getCoulombEnergy1` (`Vpbe *thee`)

Calculate coulombic energy of set of charges.
- VEXTERNC unsigned long int `Vpbe_memChk` (`Vpbe *thee`)

Return the memory used by this structure (and its contents) in bytes.

9.84.1 Detailed Description

Contains declarations for class `Vpbe`.

Version

\$Id\$

Author

Nathan A. Baker

Attention

```
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*
*

```

Definition in file [vpbe.h](#).

9.85 vpbe.h

[Go to the documentation of this file.](#)

```

00001
00066 #ifndef _VPBE_H_
00067 #define _VPBE_H_
00068
00069 #include "apbscfg.h"
00070
00071 #include "malloc/malloc.h"
00072
00073 #include "generic/vhal.h"
00074 #include "generic/vunit.h"
00075 #include "generic/vatom.h"
00076 #include "generic/vacc.h"
00077 #include "generic/vclist.h"
00078
00084 struct sVpbe {
00085
00086     Vmem *vmem;
00088     Valist *alist;
00089     Vclist *clist;
00090     Vacc *acc;
00092     double T;
00093     double soluteDiel;
00094     double solventDiel;
00095     double solventRadius;
00099     double bulkIonicStrength;
00100     double maxIonRadius;
00103     int numIon;
00104     double ionConc[MAXION];
00105     double ionRadii[MAXION];

```

```

00106     double ionQ[MAXION];
00108     double xkappa;
00109     double deblen;
00110     double zkappa2;
00111     double zmagic;
00113     double soluteCenter[3];
00114     double soluteRadius;
00115     double soluteXlen;
00116     double soluteYlen;
00117     double soluteZlen;
00118     double soluteCharge;
00120     double smvolume;
00121     double smsize;
00122     int ipkey;
00125     int paramFlag;
00127     /*-----*/
00128     /* Added by Michael Grabe */
00129     /*-----*/
00130
00131     double z_mem;
00132     double L;
00133     double membraneDiel;
00134     double V;
00135     int param2Flag;
00136     /*-----*/
00137
00138 };
00139
00144 typedef struct sVpbe Vpbe;
00145
00146 /* ////////////////////////////////////// */
00147 // Class Vpbe: Inlineable methods (vpbe.c)
00148
00149
00150 #if !defined(VINLINE_VPBE)
00151
00158 VEXTERNC Valist* Vpbe_getValist(Vpbe *thee);
00159
00166 VEXTERNC Vacc* Vpbe_getVacc(Vpbe *thee);
00167
00174 VEXTERNC double Vpbe_getBulkIonicStrength(Vpbe *thee);
00175
00182 VEXTERNC double Vpbe_getMaxIonRadius(Vpbe *thee);
00183
00190 VEXTERNC double Vpbe_getTemperature(Vpbe *thee);
00191
00198 VEXTERNC double Vpbe_getSoluteDiel(Vpbe *thee);
00199
00206 VEXTERNC double Vpbe_getGamma(Vpbe *thee);
00207
00214 VEXTERNC double Vpbe_getSoluteRadius(Vpbe *thee);
00215
00222 VEXTERNC double Vpbe_getSoluteXlen(Vpbe *thee);
00223
00230 VEXTERNC double Vpbe_getSoluteYlen(Vpbe *thee);
00231
00238 VEXTERNC double Vpbe_getSoluteZlen(Vpbe *thee);
00239
00246 VEXTERNC double* Vpbe_getSoluteCenter(Vpbe *thee);
00247
00254 VEXTERNC double Vpbe_getSoluteCharge(Vpbe *thee);
00255
00262 VEXTERNC double Vpbe_getSolventDiel(Vpbe *thee);
00263
00270 VEXTERNC double Vpbe_getSolventRadius(Vpbe *thee);
00271
00278 VEXTERNC double Vpbe_getXkappa(Vpbe *thee);
00279
00286 VEXTERNC double Vpbe_getDeblen(Vpbe *thee);
00287
00294 VEXTERNC double Vpbe_getZkappa2(Vpbe *thee);
00295
00302 VEXTERNC double Vpbe_getZmagic(Vpbe *thee);
00303
00304 /*-----*/
00305 /* Added by Michael Grabe */
00306 /*-----*/
00307
00314 VEXTERNC double Vpbe_getzmem(Vpbe *thee);
00315
00322 VEXTERNC double Vpbe_getLmem(Vpbe *thee);
00323

```

```

00330 VEXTERNC double  Vpbe_getmembraneDiel(Vpbe *thee);
00331
00337 VEXTERNC double  Vpbe_getmemv(Vpbe *thee);
00338
00339 /*-----*/
00340
00341 #else /* if defined(VINLINE_VPBE) */
00342 #   define Vpbe_getValist(thee) ((thee)->alist)
00343 #   define Vpbe_getVacc(thee) ((thee)->acc)
00344 #   define Vpbe_getBulkIonicStrength(thee) ((thee)->bulkIonicStrength)
00345 #   define Vpbe_getTemperature(thee) ((thee)->T)
00346 #   define Vpbe_getSoluteDiel(thee) ((thee)->soluteDiel)
00347 #   define Vpbe_getSoluteCenter(thee) ((thee)->soluteCenter)
00348 #   define Vpbe_getSoluteRadius(thee) ((thee)->soluteRadius)
00349 #   define Vpbe_getSoluteXlen(thee) ((thee)->soluteXlen)
00350 #   define Vpbe_getSoluteYlen(thee) ((thee)->soluteYlen)
00351 #   define Vpbe_getSoluteZlen(thee) ((thee)->soluteZlen)
00352 #   define Vpbe_getSoluteCharge(thee) ((thee)->soluteCharge)
00353 #   define Vpbe_getSolventDiel(thee) ((thee)->solventDiel)
00354 #   define Vpbe_getSolventRadius(thee) ((thee)->solventRadius)
00355 #   define Vpbe_getMaxIonRadius(thee) ((thee)->maxIonRadius)
00356 #   define Vpbe_getXkappa(thee) ((thee)->xkappa)
00357 #   define Vpbe_getDeblen(thee) ((thee)->deblen)
00358 #   define Vpbe_getZkappa2(thee) ((thee)->zkappa2)
00359 #   define Vpbe_getZmagic(thee) ((thee)->zmagic)
00360
00361 /*-----*/
00362 /* Added by Michael Grabe */
00363 /*-----*/
00364
00365 #   define Vpbe_getzmem(thee) ((thee)->z_mem)
00366 #   define Vpbe_getLmem(thee) ((thee)->L)
00367 #   define Vpbe_getmembraneDiel(thee) ((thee)->membraneDiel)
00368 #   define Vpbe_getmemv(thee) ((thee)->V)
00369
00370 /*-----*/
00371
00372
00373 #endif /* if !defined(VINLINE_VPBE) */
00374
00375 /* ////////////////////////////////////// */
00376 // Class Vpbe: Non-Inlineable methods (vpbe.c)
00377
00399 VEXTERNC Vpbe*  Vpbe_ctor(
00400     Valist *alist, /**< Atom list */
00401     int ionNum,
00402     double *ionConc,
00403     double *ionRadii,
00404     double *ionQ,
00405     double T,
00406     double soluteDiel,
00407     double solventDiel,
00408     double solventRadius,
00409     int focusFlag,
00410     double sdens,
00411     double z_mem,
00412     double L,
00413     double membraneDiel,
00414     double V
00415 );
00416
00437 VEXTERNC int  Vpbe_ctor2(
00438     Vpbe *thee,
00439     Valist *alist,
00440     int ionNum,
00441     double *ionConc,
00442     double *ionRadii,
00443     double *ionQ,
00444     double T,
00445     double soluteDiel,
00446     double solventDiel,
00447     double solventRadius,
00448     int focusFlag,
00449     double sdens,
00450     double z_mem,
00451     double L,
00452     double membraneDiel,
00453     double V
00454 );
00455
00466 VEXTERNC int  Vpbe_getIons(Vpbe *thee, int *nion, double ionConc[MAXION],

```

```

00467                                     double ionRadii[MAXION], double ionQ[MAXION]);
00468
00474 VEXTERNC void      Vpbe_dtor(Vpbe **thee);
00475
00481 VEXTERNC void      Vpbe_dtor2(Vpbe *thee);
00482
00497 VEXTERNC double    Vpbe_getCoulombEnergy1(Vpbe *thee);
00498
00506 VEXTERNC unsigned long int Vpbe_memChk(Vpbe *thee);
00507
00508 #endif /* ifndef _VPBE_H_ */

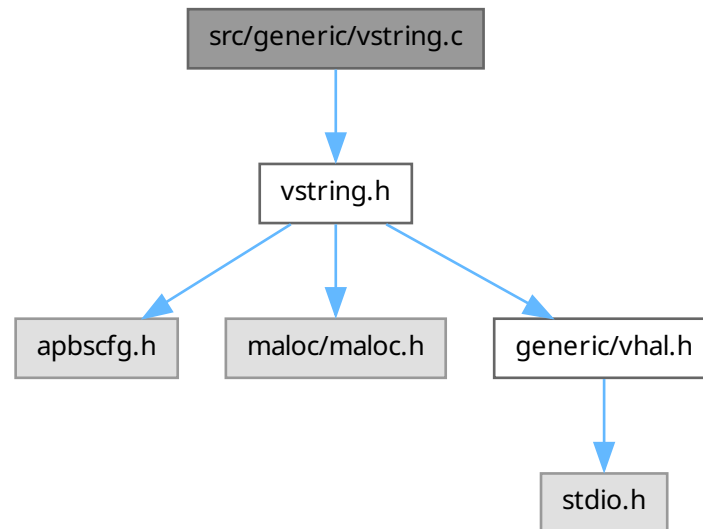
```

9.86 src/generic/vstring.c File Reference

Class Vstring methods.

```
#include "vstring.h"
```

Include dependency graph for vstring.c:



Functions

- `VPUBLIC int Vstring_strcasecmp (const char *s1, const char *s2)`
Case-insensitive string comparison (BSD standard)
- `VPUBLIC int Vstring_isdigit (const char *tok)`
A modified sscanf that examines the complete string.
- `char * Vstring_wrappedtext (const char *str, int right_margin, int left_padding)`

9.86.1 Detailed Description

Class Vstring methods.

Author

Nathan Baker

Version**Attention**

```

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*
*

```

Definition in file [vstring.c](#).

9.87 vstring.c

[Go to the documentation of this file.](#)

```

00001
00057 #include "vstring.h"
00058
00059 /* //////////////////////////////////////
```

```

00060 // Routine: Vstring_strcasecmp
00061 //
00062 //      Copyright (c) 1988-1993 The Regents of the University of
00063 //      California.
00064 //      Copyright (c) 1995-1996 Sun Microsystems, Inc.
00066 VPUBLIC int Vstring_strcasecmp(const char *s1, const char *s2) {
00067
00068     #if !defined(HAVE_STRCASECMP)
00069         unsigned char charmap[] = {
00070             0x00, 0x01, 0x02, 0x03, 0x04, 0x05, 0x06, 0x07,
00071             0x08, 0x09, 0x0a, 0x0b, 0x0c, 0x0d, 0x0e, 0x0f,
00072             0x10, 0x11, 0x12, 0x13, 0x14, 0x15, 0x16, 0x17,
00073             0x18, 0x19, 0x1a, 0x1b, 0x1c, 0x1d, 0x1e, 0x1f,
00074             0x20, 0x21, 0x22, 0x23, 0x24, 0x25, 0x26, 0x27,
00075             0x28, 0x29, 0x2a, 0x2b, 0x2c, 0x2d, 0x2e, 0x2f,
00076             0x30, 0x31, 0x32, 0x33, 0x34, 0x35, 0x36, 0x37,
00077             0x38, 0x39, 0x3a, 0x3b, 0x3c, 0x3d, 0x3e, 0x3f,
00078             0x40, 0x41, 0x42, 0x43, 0x44, 0x45, 0x46, 0x47,
00079             0x48, 0x49, 0x4a, 0x4b, 0x4c, 0x4d, 0x4e, 0x4f,
00080             0x50, 0x51, 0x52, 0x53, 0x54, 0x55, 0x56, 0x57,
00081             0x58, 0x59, 0x5a, 0x5b, 0x5c, 0x5d, 0x5e, 0x5f,
00082             0x60, 0x61, 0x62, 0x63, 0x64, 0x65, 0x66, 0x67,
00083             0x68, 0x69, 0x6a, 0x6b, 0x6c, 0x6d, 0x6e, 0x6f,
00084             0x70, 0x71, 0x72, 0x73, 0x74, 0x75, 0x76, 0x77,
00085             0x78, 0x79, 0x7a, 0x7b, 0x7c, 0x7d, 0x7e, 0x7f,
00086             0x80, 0x81, 0x82, 0x83, 0x84, 0x85, 0x86, 0x87,
00087             0x88, 0x89, 0x8a, 0x8b, 0x8c, 0x8d, 0x8e, 0x8f,
00088             0x90, 0x91, 0x92, 0x93, 0x94, 0x95, 0x96, 0x97,
00089             0x98, 0x99, 0x9a, 0x9b, 0x9c, 0x9d, 0x9e, 0x9f,
00090             0xa0, 0xa1, 0xa2, 0xa3, 0xa4, 0xa5, 0xa6, 0xa7,
00091             0xa8, 0xa9, 0xaa, 0xab, 0xac, 0xad, 0xae, 0xaf,
00092             0xb0, 0xb1, 0xb2, 0xb3, 0xb4, 0xb5, 0xb6, 0xb7,
00093             0xb8, 0xb9, 0xba, 0xbb, 0xbc, 0xbd, 0xbe, 0xbf,
00094             0xc0, 0xc1, 0xc2, 0xc3, 0xc4, 0xc5, 0xc6, 0xc7,
00095             0xc8, 0xc9, 0xca, 0xcb, 0xcc, 0xcd, 0xce, 0xcf,
00096             0xd0, 0xd1, 0xd2, 0xd3, 0xd4, 0xd5, 0xd6, 0xd7,
00097             0xd8, 0xd9, 0xda, 0xdb, 0xdc, 0xdd, 0xde, 0xdf,
00098             0xe0, 0xe1, 0xe2, 0xe3, 0xe4, 0xe5, 0xe6, 0xe7,
00099             0xe8, 0xe9, 0xea, 0xeb, 0xec, 0xed, 0xee, 0xef,
00100             0xf0, 0xf1, 0xf2, 0xf3, 0xf4, 0xf5, 0xf6, 0xf7,
00101             0xf8, 0xf9, 0xfa, 0xfb, 0xfc, 0xfd, 0xfe, 0xff,
00102         };
00103
00104         unsigned char u1, u2;
00105
00106         for ( ; ; s1++, s2++) {
00107             u1 = (unsigned char) *s1;
00108             u2 = (unsigned char) *s2;
00109             if ((u1 == '\0') || (charmap[u1] != charmap[u2])) {
00110                 break;
00111             }
00112         }
00113         return charmap[u1] - charmap[u2];
00114     #endif
00115     #else
00116         return strcasecmp(s1, s2);
00117     #endif
00118 }
00119
00120
00121
00122
00123 /* ////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////// */
00124 // Routine: Vstring_isdigit
00125 //
00126 //      Improves upon sscanf to see if a token is an int or not
00127 //
00128 //      Returns isdigit: 1 if a digit, 0 otherwise
00130 VPUBLIC int Vstring_isdigit(const char *tok) {
00131     int i, isdigit, ti;
00132     char checkchar[1];
00133     char name[VMAX_BUFSIZE];
00134     strcpy(name, tok);
00135     isdigit = 1;
00136     for(i=0; ; i++){
00137         checkchar[0] = name[i];
00138         if (name[i] == '\0'){
00139             break;
00140         }
00141         if (sscanf(checkchar, "%d", &ti) != 1){
00142             isdigit = 0;

```

```
00143         break;
00144     }
00145 }
00146 return isdigit;
00147 }
00148
00149
00155 char* Vstring_wrappedtext(const char* str, int right_margin, int left_padding)
00156 {
00157     int span = right_margin - left_padding;
00158     int i = 0;
00159     int k = 0;
00160     int j = 0;
00161     int line_len = 0;
00162     int hyphenate = 0;
00163     char* wrap_str;
00164     int wrap_len;
00165     int len = strlen( str );
00166
00167     if( len == 0 )
00168         return VNULL;
00169
00170     wrap_str = (char*)malloc( len * sizeof(char) );
00171     wrap_len = len;
00172
00173     do
00174     {
00175         if( str[i] == ' ' )
00176         {
00177             i++;
00178         }
00179         else
00180         {
00184             if( k + right_margin + 2 > wrap_len )
00185             {
00186                 wrap_len += right_margin + 2;
00187                 wrap_str = (char*)realloc( wrap_str, wrap_len * sizeof( char ) );
00188             }
00189
00190
00191             if( i + span >= len )
00192             {
00193                 hyphenate = 0;
00194                 line_len = len - i;
00195             }
00196             else
00197             {
00198                 j = span;
00199                 do
00200                 {
00201                     if( str[ i + j ] == ' ' )
00202                     {
00203                         hyphenate = 0;
00204                         line_len = j;
00205                         break;
00206                     }
00207                     else if( j == 0 )
00208                     {
00209                         hyphenate = 1;
00210                         line_len = span - 1;
00211                         break;
00212                     }
00213                     else
00214                     {
00215                         j--;
00216                     }
00217                 } while( 1 );
00218             }
00219
00220             memset( wrap_str + k, ' ', left_padding * sizeof( char ) );
00221             k += left_padding;
00222
00223             memcpy( wrap_str + k, str + i, line_len * sizeof( char ) );
00224             k += line_len;
00225             i += line_len;
00226
00227             if( hyphenate )
00228                 wrap_str[k++] = '-';
00229
00230             wrap_str[k++] = '\n';
00231         }
00232     }
```

```

00232         wrap_str[k] = '\0';
00233     }
00234     } while( i < len );
00235
00236     return wrap_str;
00237 }

```

9.88 src/generic/vstring.h File Reference

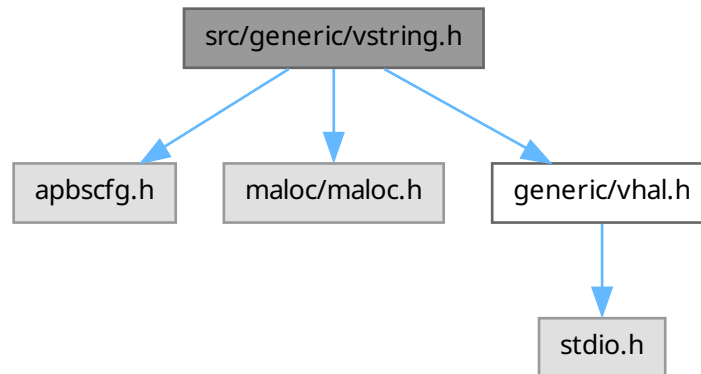
Contains declarations for class Vstring.

```

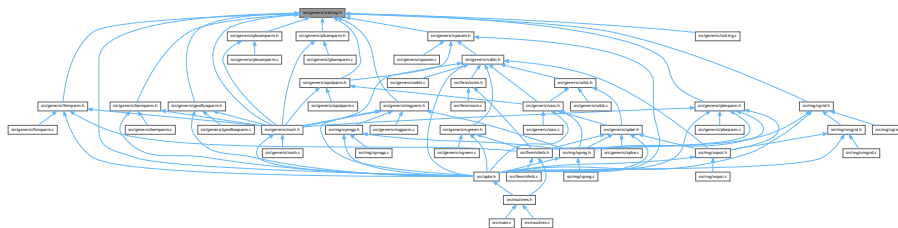
#include "apbscfg.h"
#include "maloc/maloc.h"
#include "generic/vhal.h"

```

Include dependency graph for vstring.h:



This graph shows which files directly or indirectly include this file:



Functions

- VEXTERNC int [Vstring_strcasecmp](#) (const char *s1, const char *s2)
Case-insensitive string comparison (BSD standard)
- VEXTERNC int [Vstring_isdigit](#) (const char *tok)
A modified sscanf that examines the complete string.
- char * [Vstring_wrappedtext](#) (const char *str, int right_margin, int left_padding)

9.88.1 Detailed Description

Contains declarations for class Vstring.

Version

\$Id\$

Author

Nathan A. Baker

Attention

```
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*
* Nathan A. Baker (nathan.baker@pnnl.gov)
* Pacific Northwest National Laboratory
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```


- Multiply by this to convert J to cal.*

 - #define `Vunit_cal_to_J` 2.3900574e-01
- Multiply by this to convert cal to J.*

 - #define `Vunit_amu_to_kg` 1.6605402e-27
- Multiply by this to convert amu to kg.*

 - #define `Vunit_kg_to_amu` 6.0221367e+26
- Multiply by this to convert kg to amu.*

 - #define `Vunit_ec_to_C` 1.6021773e-19
- Multiply by this to convert ec to C.*

 - #define `Vunit_C_to_ec` 6.2415065e+18
- Multiply by this to convert C to ec.*

 - #define `Vunit_ec` 1.6021773e-19
- Charge of an electron in C.*

 - #define `Vunit_kb` 1.3806581e-23
- Boltzmann constant.*

 - #define `Vunit_Na` 6.0221367e+23
- Avogadro's number.*

 - #define `Vunit_pi` VPI
- Pi.*

 - #define `Vunit_eps0` 8.8541878e-12
- Vacuum permittivity.*

 - #define `Vunit_esu_ec2A` 3.3206364e+02
- e_c^2 / in ESU units => kcal/mol*

 - #define `Vunit_esu_kb` 1.9871913e-03
- k_b in ESU units => kcal/mol*

9.90.1 Detailed Description

Contains a collection of useful constants and conversion factors.

Author

Nathan Baker
Nathan A. Baker

Version

\$Id\$

Attention

```
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*
* Nathan A. Baker (nathan.baker@pnnl.gov)
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*
*

```

Definition in file [vunit.h](#).

9.91 vunit.h

[Go to the documentation of this file.](#)

```

00001
00063 #ifndef _VUNIT_H_
00064 #define _VUNIT_H_
00065
00068 #define Vunit_J_to_cal 4.1840000e+00
00069
00072 #define Vunit_cal_to_J 2.3900574e-01
00073
00076 #define Vunit_amu_to_kg 1.6605402e-27
00077
00080 #define Vunit_kg_to_amu 6.0221367e+26
00081
00084 #define Vunit_ec_to_C 1.6021773e-19
00085
00088 #define Vunit_C_to_ec 6.2415065e+18
00089
00092 #define Vunit_ec 1.6021773e-19
00093
00096 #define Vunit_kb 1.3806581e-23
00097
00100 #define Vunit_Na 6.0221367e+23
00101
00104 #define Vunit_pi VPI
00105
00108 #define Vunit_eps0 8.8541878e-12
00109
00112 #define Vunit_esu_ec2A 3.3206364e+02
00113
00116 #define Vunit_esu_kb 1.9871913e-03
00117
00118 #endif /* ifndef _VUNIT_H_ */

```

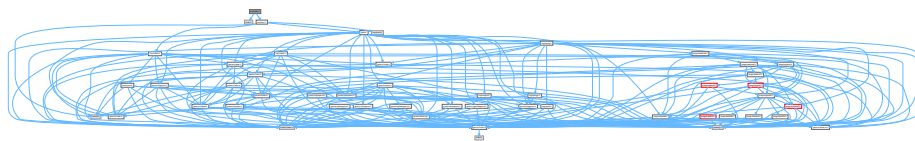
9.92 src/main.c File Reference

APBS "front end" program using formatted input files.

```
#include <time.h>
```

```
#include "routines.h"
```

Include dependency graph for main.c:



Functions

- int [main](#) (int argc, char **argv)

The main APBS function.

9.92.1 Detailed Description

APBS "front end" program using formatted input files.

Author

Nathan Baker

This driver program represents a mish-mash of instructions for calculating electrostatic potentials, as well as free energies of binding and solvation. It is invoked as:

```
apbs apbs.in
```

where apbs.in is a formatted input file (see documentation and examples).

Version

\$Id\$

Attention

```
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*
* Nathan A. Baker (nathan.baker@pnnl.gov)
* Pacific Northwest National Laboratory
*
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```

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*
*

```

Definition in file [main.c](#).

9.93 main.c

[Go to the documentation of this file.](#)

```

00001
00068 #include <time.h>
00069
00070 #include "routines.h"
00071
00072 VEMBED(rcsid="$Id$")
00073
00074
00080 int main(
00081     int argc,
00082     char **argv
00083 )
00084 {
00085     // PCE: Adding below variables temporarily
00086     clock_t ts, te;
00087     // End PCE
00088
00089     NOsh *nosh = VNULL;
00090
00091     MGparm *mgparm = VNULL;
00092     FEMparm *feparm = VNULL;
00093 #ifdef ENABLE_BEM
00094     BEMparm *beparm = VNULL;
00095 #endif
00096     GEOWflowparm *geowflowparm = VNULL;
00097     PBEparm *pbeparm = VNULL;
00098     APOLparm *apolparm = VNULL;
00099     Vparam *param = VNULL;
00100 #if defined(ENABLE_PBAM) || defined(ENABLE_PBSAM)
00101     PBAMparm *pbamparm = VNULL;
00102 #endif
00103
00104 #ifdef ENABLE_PBSAM
00105     PBSAMparm *pbsamparm = VNULL;
00106 #endif
00107
00108     Vmem *mem = VNULL;
00109     Vcom *com = VNULL;
00110     Vio *sock = VNULL;

```

```

00111 #ifdef HAVE_MC_H
00112     Vfetk *fetk[NOSH_MAXCALC];
00113     Gem *gm[NOSH_MAXMOL];
00114     int isolve;
00115 #else
00116     void *fetk[NOSH_MAXCALC];
00117     void *gm[NOSH_MAXMOL];
00118 #endif
00119     Vpmg *pmg[NOSH_MAXCALC];
00120     Vpmgp *pmgp[NOSH_MAXCALC];
00121     Vpbe *pbe[NOSH_MAXCALC];
00122     Valist *alist[NOSH_MAXMOL];
00123     Vgrid *dielXMap[NOSH_MAXMOL],
00124           *dielYMap[NOSH_MAXMOL],
00125           *dielZMap[NOSH_MAXMOL],
00126           *kappaMap[NOSH_MAXMOL],
00127           *potMap[NOSH_MAXMOL],
00128           *chargeMap[NOSH_MAXMOL];
00129     char *input_path = VNULL,
00130          *output_path = VNULL;
00131     int i,
00132         rank,    // proc id
00133         size,    // total num of procs
00134         k;
00135     size_t bytesTotal,
00136           highWater;
00137     Voutput_Format outputformat;
00138
00139     int rc = 0;
00140
00141     /* The energy double arrays below store energies from various calculations. */
00142     double qfEnergy[NOSH_MAXCALC],
00143            qmEnergy[NOSH_MAXCALC];
00144     double dielEnergy[NOSH_MAXCALC],
00145            totEnergy[NOSH_MAXCALC];
00146     double *atomEnergy[NOSH_MAXCALC];
00147     AtomForce *atomForce[NOSH_MAXCALC]; /* Stores forces from various calculations. */
00148     int nenergy[NOSH_MAXCALC], /* Stores either a flag (0,1) displaying whether
00149                                * energies were calculated, or, if PCE_COMPS
00150                                * was used, the number of atom energies stored
00151                                * for the given calculation. */
00152         nforce[NOSH_MAXCALC]; /* Stores an integer which either says no
00153                                * calculation was performed (0) or gives the
00154                                * number of entries in the force array for each
00155                                * calculation. */
00156
00157     /* The real partition centers */
00158     double realCenter[3];
00159
00160     /* Instructions: */
00161     char header[] = {"\n\n\
00162 -----\n\
00163 APBS -- Adaptive Poisson-Boltzmann Solver\n\
00164 Version " PACKAGE_STRING "\n\
00165 \n\
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00167 Pacific Northwest National Laboratory\n\
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00204     SOFTWARE, EVEN IF ADVISED OF THE POSSIBILITY OF SUCH DAMAGE.\n\
00205     ----- \n\
00206     APBS uses FETK (the Finite Element ToolKit) to solve the\n\
00207     Poisson-Boltzmann equation numerically. FETK is a portable collection\n\
00208     of finite element modeling class libraries developed by the Michael Holst\n\
00209     research group and written in an object-oriented form of C. FETk is\n\
00210     designed to solve general coupled systems of nonlinear partial differential\n\
00211     equations using adaptive finite element methods, inexact Newton methods,\n\
00212     and algebraic multilevel methods. More information about FETk may be found\n\
00213     at <http://www.FETk.ORG>.\n\
00214     ----- \n\
00215     APBS also uses Aqua to solve the Poisson-Boltzmann equation numerically. \n\
00216     Aqua is a modified form of the Holst group PMG library <http://www.FETk.ORG>\n\
00217     which has been modified by Patrice Koehl\n\
00218     <http://koehlhab.genomecenter.ucdavis.edu/> for improved efficiency and\n\
00219     memory usage when solving the Poisson-Boltzmann equation.\n\
00220     ----- \n\
00221     Please cite your use of APBS as:\n\
00222     Baker NA, Sept D, Joseph S, Holst MJ, McCammon JA. Electrostatics of\n\
00223     nanosystems: application to microtubules and the ribosome. Proc.\n\
00224     Natl. Acad. Sci. USA 98, 10037-10041 2001.\n\
00225     \n\n");
00226     char *usage =
00227     {"\n\n\
00228     ----- \n\
00229     This driver program calculates electrostatic potentials, energies,\n\
00230     and forces using both multigrid and finite element methods.\n\
00231     It is invoked as:\n\
00232     apbs [options] apbs.in\n\
00233     where apbs.in is a formatted input file and [options] are:\n\
00234     --output-file=<name>    Enables output logging to the path\n\
00235     listed in <name>. Uses flat-file\n\
00236     format is --output-format is not used.\n\
00237     --output-format=<type>  Specifies format for logging. Options\n\
00238     for type are either \"xml\" or \"flat\".\n\
00239     --help                  Display this help information.\n\
00240     --version               Display the current APBS version.\n\
00241     ----- \n\n");
00242
00243     /* ***** CHECK PARALLEL STATUS ***** */
00244     VASSERT(Vcom_init(&argc, &argv));
00245     com = Vcom_ctor(1);
00246     rank = Vcom_rank(com);
00247     size = Vcom_size(com);
00248     startVio();
00249     Vnm_setIoTag(rank, size);
00250     Vnm_tprint( 0, "Hello world from PE %d\n", rank);
00251
00252     /* A bit of array/pointer initialization */
00253     mem = Vmem_ctor("MAIN");
00254     for (i=0; i<NOSH_MAXCALC; i++) {
00255         pmg[i] = VNULL;
00256         pmgp[i] = VNULL;
00257         fetk[i] = VNULL;
00258         pbe[i] = VNULL;
00259         qfEnergy[i] = 0;
00260         qmEnergy[i] = 0;
00261         dielEnergy[i] = 0;
00262         totEnergy[i] = 0;
00263         atomForce[i] = VNULL;
00264         nenergy[i] = 0;
00265         nforce[i] = 0;
00266     }
00267     for (i=0; i<NOSH_MAXMOL; i++) {
00268         alist[i] = VNULL;
00269         dielXMap[i] = VNULL;
00270         dielYMap[i] = VNULL;
00271         dielZMap[i] = VNULL;
00272         kappaMap[i] = VNULL;

```



```

00273         potMap[i] = VNULL;
00274         chargeMap[i] = VNULL;
00275     }
00276
00277     /* ***** CHECK INVOCATION AND OPTIONS ***** */
00278     Vnm_tstart(APBS_TIMER_WALL_CLOCK, "APBS WALL CLOCK");
00279     Vnm_tprint( 1, "%s", header);
00280
00281 #ifdef APBS_FAST
00282     Vnm_tprint(, 2"WARNING: APBS was compiled with the --enable-fast option.\n"
00283         "WARNING: This mode is experimental and subject to change in future releases.\n"
00284         "WARNING: The fast mode enables: Gauss-Seidel Smoothing and \n"
00285         "WARNING: Conjugate Gradient Multigrid methods.\n\n");
00286 #endif
00287
00288     Vnm_tprint( 1, "This executable compiled on %s at %s\n\n", __DATE__, __TIME__);
00289
00290 #if defined(WITH_TINKER)
00291     Vnm_tprint( 2, "This executable was compiled with TINKER support and is not intended for stand-alone
00292     execution.\n");
00293     Vnm_tprint( 2, "Please compile another version without TINKER support.\n");
00294     exit(2);
00295 #endif
00296
00297     /* Process program arguments */
00298     i=0;
00299     outputformat = OUTPUT_NULL;
00300     while (i<argc){
00301         if (strncmp(argv[i], "--", 2) == 0) {
00302             /* Long Options */
00303             if (Vstring_strcasecmp("--version", argv[i]) == 0){
00304                 Vnm_tprint(2, "%s\n", PACKAGE_STRING);
00305                 VJMPERR1(0);
00306             } else if (Vstring_strcasecmp("--help", argv[i]) == 0){
00307                 Vnm_tprint(2, "%s\n", usage);
00308                 VJMPERR1(0);
00309             } else if (strncmp(argv[i], "--output-format", 15) == 0) {
00310                 if (strstr(argv[i], "xml") != NULL) {
00311                     Vnm_tprint(2, "XML output format is now deprecated, please use --output-format=flat
00312                     instead!\n\n");
00313                     VJMPERR1(0);
00314                 }
00315                 else if (strstr(argv[i], "flat") != NULL) {
00316                     outputformat = OUTPUT_FLAT;
00317                 } else {
00318                     Vnm_tprint(2, "Invalid output-format type!\n");
00319                     VJMPERR1(0);
00320                 }
00321             } else if (strncmp(argv[i], "--output-file=", 14) == 0){
00322                 output_path = strstr(argv[i], "=");
00323                 ++output_path;
00324                 if (outputformat == OUTPUT_NULL) outputformat = OUTPUT_FLAT;
00325             } else {
00326                 Vnm_tprint(2, "UNRECOGNIZED COMMAND LINE OPTION %s!\n", argv[i]);
00327                 Vnm_tprint(2, "%s\n", usage);
00328                 VJMPERR1(0);
00329             }
00330         } else {
00331             /* Set the path to the input file */
00332             if ((input_path == VNULL) && (i != 0))
00333                 input_path = argv[i];
00334             else if (i != 0) {
00335                 Vnm_tprint(2, "ERROR -- CALLED WITH TOO MANY ARGUMENTS!\n", \
00336                     argc);
00337                 Vnm_tprint(2, "%s\n", usage);
00338                 VJMPERR1(0);
00339             }
00340         }
00341         i++;
00342     }
00343
00344     /* If we set an output format but no path, error. */
00345     if ((outputformat != 0) && (output_path == NULL)) {
00346         Vnm_tprint(2, "The --output-path variable must be set when using --output-format!\n");
00347         VJMPERR1(0);
00348     }
00349
00350     /* If we failed to specify an input file, error. */
00351     if (input_path == NULL) {

```

```

00352     Vnm_tprint(2, "ERROR -- APBS input file not specified!\n", argc);
00353     Vnm_tprint(2, "%s\n", usage);
00354     VJMPERR1(0);
00355 }
00356
00357 /* Append rank info if a parallel run */
00358 if ((size > 1) && (output_path != NULL))
00359     printf(output_path, "%s%d", output_path, rank);
00360
00361 /* ***** PARSE INPUT FILE ***** */
00362 nosh = Nosh_ctor(rank, size);
00363 Vnm_tprint( 1, "Parsing input file %s...\n", input_path);
00364 Vnm_tprint( 1, "rank %d size %d...\n", rank, size);
00365 sock = Vio_ctor("FILE", "ASC", VNULL, input_path, "r");
00366 if (sock == VNULL) {
00367     Vnm_tprint(2, "Error while opening input file %s!\n", input_path);
00368     VJMPERR1(0);
00369 }
00370 if (!Nosh_parseInput(nosh, sock)) {
00371     Vnm_tprint( 2, "Error while parsing input file.\n");
00372     VJMPERR1(0);
00373 }
00374 else
00375     Vnm_tprint( 1, "Parsed input file.\n");
00376 Vio_dtor(&sock);
00377
00378 /* ***** LOAD PARAMETERS AND MOLECULES ***** */
00379 param = loadParameter(nosh);
00380 if (loadMolecules(nosh, param, alist) != 1) {
00381     Vnm_tprint(2, "Error reading molecules!\n");
00382     VJMPERR1(0);
00383 }
00384
00385 /* ***** SETUP CALCULATIONS ***** */
00386 if (Nosh_setupElecCalc(nosh, alist) != 1) {
00387     Vnm_tprint(2, "Error setting up ELEC calculations\n");
00388     VJMPERR1(0);
00389 }
00390
00391 if ((rc = Nosh_setupApolCalc(nosh, alist)) == ACD_ERROR) {
00392     Vnm_tprint(2, "Error setting up APOL calculations\n");
00393     VJMPERR1(0);
00394 }
00395
00396 /* ***** CHECK APOL***** */
00397 /* if((nosh->gotparm == 0) && (rc == ACD_YES)){
00398     Vnm_print(1, "\nError you must provide a parameter file if you\n" \
00399             "are performing an APOLAR calculation\n");
00400     VJMPERR1(0);
00401 } */
00402
00403 #if defined(DEBUG_MAC_OSX_OCL)
00404 #include "mach_chud.h"
00405 #include <stdint.h>
00406 uint64_t mbeg;
00407 machm_(&mbeg);
00408
00409 if(clFinish != NULL)
00410 {
00411     int ret = initOpenCL();
00412     printf("OpenCL runtime present - initialized = %i\n",ret);
00413 }
00414 else
00415 {
00416     setkOpenCLAvailable_(0);
00417     printf("OpenCL is not present!\n");
00418 }
00419 #endif
00420
00421 #if defined(DEBUG_MAC_OSX_STANDARD)
00422 #include "mach_chud.h"
00423 #include <stdint.h>
00424 uint64_t mbeg;
00425 machm_(&mbeg);
00426 #endif
00427
00428 /* ***** LOAD MAPS ***** */
00429 if (loadDielMaps(nosh, dielXMap, dielYMap, dielZMap) != 1) {
00430     Vnm_tprint(2, "Error reading dielectric maps!\n");
00431     VJMPERR1(0);
00432 }

```

```

00433     if (loadKappaMaps(nosh, kappaMap) != 1) {
00434         Vnm_tprint(2, "Error reading kappa maps!\n");
00435         VJMPERR1(0);
00436     }
00437     if (loadPotMaps(nosh, potMap) != 1) {
00438         Vnm_tprint(2, "Error reading potential maps!\n");
00439         VJMPERR1(0);
00440     }
00441     if (loadChargeMaps(nosh, chargeMap) != 1) {
00442         Vnm_tprint(2, "Error reading charge maps!\n");
00443         VJMPERR1(0);
00444     }
00445
00446     /* ***** DO THE CALCULATIONS ***** */
00447     Vnm_tprint(1, "Preparing to run %d PBE calculations.\n",
00448         nosh->ncalc);
00449     for (i=0; i<nosh->ncalc; i++) {
00450         Vnm_tprint(1, "-----\n");
00451
00452         switch (nosh->calc[i]->calctype) {
00453             /* Multigrid */
00454             case NCT_MG:
00455                 /* What is this? This seems like a very awkward way to find
00456                    the right ELEC statement... */
00457                 for (k=0; k<nosh->nelec; k++) {
00458                     if (nosh->elec2calc[k] >= i) {
00459                         break;
00460                     }
00461                 }
00462                 if (Vstring_strcasecmp(nosh->elecname[k], "") == 0) {
00463                     Vnm_tprint(1, "CALCULATION #d: MULTIGRID\n", i+1);
00464                 } else {
00465                     Vnm_tprint(1, "CALCULATION #d (%s): MULTIGRID\n",
00466                         i+1, nosh->elecname[k]);
00467                 }
00468                 /* Useful local variables */
00469                 mgparm = nosh->calc[i]->mgparm;
00470                 pbeparm = nosh->calc[i]->pbeparm;
00471
00472                 /* Set up problem */
00473                 Vnm_tprint(1, "Setting up problem...\n");
00474
00475                 if (!initMG(i, nosh, mgparm, pbeparm, realCenter, pbe,
00476                     alist, dielXMap, dielYMap, dielZMap, kappaMap,
00477                     chargeMap, pmgp, pmg, potMap)) {
00478                     Vnm_tprint(2, "Error setting up MG calculation!\n");
00479                     VJMPERR1(0);
00480                 }
00481
00482                 /* Print problem parameters */
00483                 printMGPARAM(mgparm, realCenter);
00484                 printPBEPARM(pbeparm);
00485
00486                 /* Solve PDE */
00487                 if (solveMG(nosh, pmg[i], mgparm->type) != 1) {
00488                     Vnm_tprint(2, "Error solving PDE!\n");
00489                     VJMPERR1(0);
00490                 }
00491
00492                 /* Set partition information for observables and I/O */
00493                 if (setPartMG(nosh, mgparm, pmg[i]) != 1) {
00494                     Vnm_tprint(2, "Error setting partition info!\n");
00495                     VJMPERR1(0);
00496                 }
00497
00498                 /* Write out energies */
00499                 energyMG(nosh, i, pmg[i],
00500                     &(nenergy[i]), &(totEnergy[i]), &(qfEnergy[i]),
00501                     &(qmEnergy[i]), &(dielEnergy[i]));
00502
00503                 /* Write out forces */
00504                 forceMG(mem, nosh, pbeparm, mgparm, pmg[i], &(nforce[i]),
00505                     &(atomForce[i]), alist);
00506
00507                 /* Write out data folks might want */
00508                 writedataMG(rank, nosh, pbeparm, pmg[i]);
00509
00510                 /* Write matrix */
00511                 writematMG(rank, nosh, pbeparm, pmg[i]);
00512
00513                 /* If needed, cache atom energies */

```

```

00514         nenergy[i] = 0;
00515         if ((pbeparm->calcenergy == PCE_COMPS) && (outputformat != OUTPUT_NULL)){
00516             storeAtomEnergy(pmg[i], i, &(atomEnergy[i]), &(nenergy[i]));
00517         }
00518
00519         fflush(stdout);
00520         fflush(stderr);
00521
00522         break;
00523
00524         /* ***** Do FEM calculation ***** */
00525         case NCT_FEM:
00526 #ifdef HAVE_MC_H
00527         for (k=0; k<nosh->nelec; k++) {
00528             if (nosh->elec2calc[k] >= i) break;
00529         }
00530         if (Vstring_strcasecmp(nosh->elecname[i+1], "") == 0) {
00531             Vnm_tprint( 1, "CALCULATION #d: FINITE ELEMENT\n", i+1);
00532         } else {
00533             Vnm_tprint( 1, "CALCULATION #d (%s): FINITE ELEMENT\n", i+1, nosh->elecname[k+1]);
00534         }
00535
00536         /* Useful local variables */
00537         feparm = nosh->calc[i]->feparm;
00538         pbeparm = nosh->calc[i]->pbeparm;
00539
00540         /* Warn the user about some things */
00541         Vnm_tprint(2, "##### WARNING #####\n");
00542         Vnm_tprint(2, "## FE support is currently very experimental! ##\n");
00543         Vnm_tprint(2, "##### WARNING #####\n");
00544
00545         /* Set up problem */
00546         Vnm_tprint( 1, "    Setting up problem...\n");
00547         /* Attempt to initialize and do an initial refinement of the mesh data. The mesh data
00548          * will be stored in the Vfetk object fetk, which contains the appropriate geometry
00549          * manager (Gem) object and Vcsm object describing the mesh structure. The mesh will
00550          * either be loaded from an external source or generated from scratch. */
00551         if (initFE(i, nosh, feparm, pbeparm, pbe, alist, fetk) != VRC_SUCCESS) {
00552             Vnm_tprint( 2, "Error setting up FE calculation!\n");
00553             VJMERR1(0);
00554         }
00555
00556         /* Print problem parameters */
00557         printFEPARM(i, nosh, feparm, fetk);
00558         printPBEPARM(pbeparm);
00559
00560         /* Refine mesh - this continues to run the AM_markRefine procedure already run
00561          * in initFE() to arrive at some initial refinement, but does checks of the
00562          * simplices so that it refines until the error or size tolerances are reached.
00563          * Once this is done, we have a mesh that has been refined to the point where
00564          * we can attempt to solve - further refinement may be needed in the loop
00565          * below. */
00566         if (!preRefineFE(i, feparm, fetk)) {
00567             Vnm_tprint( 2, "Error pre-refining mesh!\n");
00568             VJMERR1(0);
00569         }
00570
00571         /* Solve-estimate-refine */
00572         Vnm_tprint(2, "\n\nWARNING! DO NOT EXPECT PERFORMANCE OUT OF THE APBS/FETk\n");
00573         Vnm_tprint(2, "INTERFACE AT THIS TIME. THE FINITE ELEMENT SOLVER IS\n");
00574         Vnm_tprint(2, "CURRENTLY NOT OPTIMIZED FOR THE PB EQUATION. IF YOU WANT\n");
00575         Vnm_tprint(2, "PERFORMANCE, PLEASE USE THE MULTIGRID-BASED METHODS, E.G.\n");
00576         Vnm_tprint(2, "MG-AUTO, MG-PARA, and MG-MANUAL (SEE DOCS.)\n\n");
00577         Vnm_tprint(1, "    Beginning solve-estimate-refine cycle:\n");
00578
00579         for (isolve=0; isolve<feparm->maxsolve; isolve++) {
00580             Vnm_tprint(1, "        Solve #d...\n", isolve);
00581
00582             /* Attempt to solve the mesh by using one of MC's solver types. */
00583             if (!solveFE(i, pbeparm, feparm, fetk)) {
00584                 Vnm_tprint(2, "ERROR SOLVING EQUATION!\n");
00585                 VJMERR1(0);
00586             }
00587
00588             /* Calculate the total electrostatic energy. */
00589             if (!energyFE(nosh, i, fetk, &(nenergy[i]),
00590                 &(totEnergy[i]), &(qfEnergy[i]),
00591                 &(qmEnergy[i]), &(dielEnergy[i]))) {
00592                 Vnm_tprint(2, "ERROR SOLVING EQUATION!\n");
00593                 VJMERR1(0);
00594             }

```

```

00595
00596         /* We're not going to refine if we've hit the max number
00597         * of solves */
00598         if (isolve < (feparm->maxsolve)-1) {
00599             /* Do a final error estimation and mesh refinement. */
00600             if (!postRefineFE(i, feparm, fetk)) {
00601                 break;
00602             }
00603         }
00604         bytesTotal = Vmem_bytesTotal();
00605         highWater = Vmem_highWaterTotal();
00606         Vnm_tprint(1, "      Current memory use:      %g MB\n",
00607             ((double)bytesTotal/(1024.)/(1024.)));
00608         Vnm_tprint(1, "      High-water memory use:  %g MB\n",
00609             ((double)highWater/(1024.)/(1024.)));
00610     }
00611
00612     Vnm_tprint(1, "  Writing FEM data to files.\n");
00613
00614     /* Save data. */
00615     if (!writedataFE(rank, nosh, pbeparm, fetk[i])) {
00616         Vnm_tprint(2, "  Error while writing FEM data!\n");
00617     }
00618 #else /* ifdef HAVE_MC_H */
00619     Vnm_print(2, "Error!  APBS not compiled with FETk!\n");
00620     exit(2);
00621 #endif /* ifdef HAVE_MC_H */
00622     break;
00623
00624     /* Do an apolar calculation */
00625     case NCT_APOL:
00626         /* Copied from NCT_MG. See the note above (top of loop) for
00627         information about this loop.
00628         */
00629         for (k=0; k<nosh->napol; k++) {
00630             if (nosh->apol2calc[k] >= i) {
00631                 break;
00632             }
00633         }
00634
00635         if (Vstring_strcasecmp(nosh->apolname[k], "") == 0) {
00636             Vnm_tprint( 1, "CALCULATION #d: APOLAR\n", i+1);
00637         } else {
00638             Vnm_tprint( 1, "CALCULATION #d (%s): APOLAR\n",
00639                 i+1, nosh->apolname[k]);
00640         }
00641
00642         apolparm = nosh->calc[i]->apolparm;
00643         // poor man's execution timer.
00644         ts = clock();
00645         rc = initAPOL(nosh, mem, param, apolparm, &(nforce[i]), &(atomForce[i]),
00646             alist[(apolparm->molid)-1]);
00647         Vnm_print(0, "initAPOL: Time elapsed: %f\n", ((double)clock() - ts) / CLOCKS_PER_SEC);
00648         if (rc == 0) {
00649             Vnm_tprint(2, "Error calculating apolar solvation quantities!\n");
00650             VJMPErr(0);
00651         }
00652         break;
00653
00654     /* Boundary Element (tabi) */
00655     case NCT_BEM:
00656 #ifdef ENABLE_BEM
00657         /* What is this? This seems like a very awkward way to find
00658         the right ELEC statement... */
00659         for (k=0; k<nosh->nelec; k++) {
00660             if (nosh->elec2calc[k] >= i) {
00661                 break;
00662             }
00663         }
00664         if (Vstring_strcasecmp(nosh->elecname[k], "") == 0) {
00665             Vnm_tprint( 1, "CALCULATION #d: BOUNDARY ELEMENT\n", i+1);
00666         } else {
00667             Vnm_tprint( 1, "CALCULATION #d (%s): BOUNDARY ELEMENT\n",
00668                 i+1, nosh->elecname[k]);
00669         }
00670         /* Useful local variables */
00671         bemparm = nosh->calc[i]->bemparm;
00672         pbeparm = nosh->calc[i]->pbeparm;
00673
00674         /* Set up problem */
00675         Vnm_tprint( 1, "  Setting up problem...\n");

```

```

00676
00677         if (!initBEM(i,nosh, bemparm, pbeparm, pbe)) {
00678             Vnm_tprint( 2, "Error setting up BEM calculation!\n");
00679             VJMPERR1(0);
00680         }
00681
00682         /* Print problem parameters */
00683         printBEMPARM(bemparm);
00684         printPBEPARM(pbeparm);
00685
00686         /* Solve PDE */
00687         if (solveBEM(alist, nosh, pbeparm, bemparm, bemparm->type) != 1) {
00688             Vnm_tprint(2, "Error solving PDE!\n");
00689             VJMPERR1(0);
00690         }
00691
00692         /* Write out energies */
00693         energyBEM(nosh, i,
00694                 &(nenergy[i]), &(totEnergy[i]), &(qfEnergy[i]),
00695                 &(qmEnergy[i]), &(dielEnergy[i]));
00696
00697         /* Write out forces */
00698         forceBEM(nosh, pbeparm, bemparm, &(nforce[i]),
00699                 &(atomForce[i]), alist);
00700
00701         /* Write out data folks might want */
00702         writedataBEM(rank, nosh, pbeparm);
00703
00704         /* Write matrix */
00705         writematBEM(rank, nosh, pbeparm);
00706
00707         /* If needed, cache atom energies */
00708         nenergy[i] = 0;
00709         if ((pbeparm->calcenergy == PCE_COMPS) && (outputformat != OUTPUT_NULL)){
00710             storeAtomEnergy(pmg[i], i, &(atomEnergy[i]), &(nenergy[i]));
00711         }
00712
00713         fflush(stdout);
00714         fflush(stderr);
00715     #else /* ifdef ENABLE_BEM */
00716         Vnm_tprint(2, "Error! APBS not compiled with BEM!\n");
00717         exit(2);
00718     #endif
00719     break;
00720
00721     /* geometric flow */
00722     case NCT_GEOFLOW:
00723     #ifdef ENABLE_GEOFLOW
00724         /* What is this? This seems like a very awkward way to find
00725         the right ELEC statement... */
00726         for (k=0; k<nosh->nelec; k++) {
00727             if (nosh->elec2calc[k] >= i) {
00728                 break;
00729             }
00730         }
00731         if (Vstring_strcasecmp(nosh->elecname[k], "") == 0) {
00732             Vnm_tprint( 1, "CALCULATION #d: GEOMETRIC FLOW\n", i+1);
00733         } else {
00734             Vnm_tprint( 1, "CALCULATION #d (%s): GEOMETRIC FLOW\n",
00735                 i+1, nosh->elecname[k]);
00736         }
00737         /* Useful local variables */
00738         geoflowparm = nosh->calc[i]->geoflowparm;
00739         apolparm = nosh->calc[i]->apolparm;
00740         pbeparm = nosh->calc[i]->pbeparm;
00741
00742         /* Set up problem */
00743         Vnm_tprint( 1, " Setting up problem...\n");
00744
00745
00746         /* Solve PDE */
00747         if (solveGeometricFlow(alist, nosh, pbeparm, apolparm, geoflowparm) != 1) {
00748             Vnm_tprint(2, "Error solving GEOFLOW!\n");
00749             VJMPERR1(0);
00750         }
00751
00752         fflush(stdout);
00753         fflush(stderr);
00754         break;
00755     #else /* ifdef ENABLE_GEOFLOW */
00756         Vnm_tprint(2, "Error! APBS not compiled with GEOFLOW!\n");

```

```

00757             exit(2);
00758 #endif
00759
00760         /* Poisson-boltzmann analytical method */
00761         case NCT_PBAM:
00762 #ifdef ENABLE_PBAM
00763             /* What is this? This seems like a very awkward way to find
00764             the right ELEC statement... */
00765             //Vnm_tprint( 1, "Made it to start\n");
00766             for (k=0; k<nosh->nelec; k++) {
00767                 if (nosh->elec2calc[k] >= i) {
00768                     break;
00769                 }
00770             }
00771             if (Vstring_strcasecmp(nosh->elecname[k], "") == 0) {
00772                 Vnm_tprint( 1, "CALCULATION #d: PBAM\n", i+1);
00773             } else {
00774                 Vnm_tprint( 1, "CALCULATION #d (%s): PBAM\n",
00775                     i+1, nosh->elecname[k]);
00776             }
00777             /* Useful local variables */
00778             pbamparm = nosh->calc[i]->pbamparm;
00779             pbeparm = nosh->calc[i]->pbeparm;
00780
00781             /* Set up problem */
00782             Vnm_tprint( 1, " Setting up problem...\n");
00783
00784             /* Solve LPBE with PBAM method */
00785             if (solvePBAM(alist, nosh, pbeparm, pbamparm) != 1) {
00786                 Vnm_tprint(2, "Error solving PBAM!\n");
00787                 VJMPERR1(0);
00788             }
00789
00790             fflush(stdout);
00791             fflush(stderr);
00792             break;
00793 #else /* ifdef ENABLE_PBAM */
00794             Vnm_print(2, "Error! APBS not compiled with PBAM!\n");
00795             exit(2);
00796 #endif
00797
00798         case NCT_PBSAM:
00799 #ifdef ENABLE_PBSAM
00800             Vnm_tprint( 1, "Made it to start\n");
00801             for (k=0; k<nosh->nelec; k++) {
00802                 if (nosh->elec2calc[k] >= i) {
00803                     break;
00804                 }
00805             }
00806             if (Vstring_strcasecmp(nosh->elecname[k], "") == 0) {
00807                 Vnm_tprint( 1, "CALCULATION #d: PBSAM\n", i+1);
00808             } else {
00809                 Vnm_tprint( 1, "CALCULATION #d (%s): PBSAM\n",
00810                     i+1, nosh->elecname[k]);
00811             }
00812             /* Useful local variables */
00813             pbamparm = nosh->calc[i]->pbamparm;
00814             pbsamparm = nosh->calc[i]->pbsamparm;
00815             pbeparm = nosh->calc[i]->pbeparm;
00816
00817             /* Set up problem */
00818             Vnm_tprint( 1, " Setting up problem...\n");
00819
00820             /* Solve LPBE with PBSAM method */
00821             if (solvePBSAM(alist, nosh, pbeparm, pbamparm, pbsamparm) != 1) {
00822                 Vnm_tprint(2, "Error solving PBSAM!\n");
00823                 VJMPERR1(0);
00824             }
00825
00826             fflush(stdout);
00827             fflush(stderr);
00828             break;
00829 #else /* ifdef ENABLE_PBSAM */
00830             Vnm_print(2, "Error! APBS not compiled with PBSAM!\n");
00831             exit(2);
00832 #endif
00833
00834         default:
00835             Vnm_tprint(2, " Unknown calculation type (%d)!\n", nosh->calc[i]->calctype);
00836             exit(2);
00837

```

```

00838         break;
00839     }
00840 }
00841 }
00842
00843 //Clear out the parameter file memory
00844 if(param != VNULL) Vparam_dtor(&param);
00845
00846 /* ***** HANDLE PRINT STATEMENTS ***** */
00847 if (nosh->nprint > 0) {
00848     Vnm_tprint( 1, "-----\n");
00849     Vnm_tprint( 1, "PRINT STATEMENTS\n");
00850 }
00851 for (i=0; i<nosh->nprint; i++) {
00852     /* Print energy */
00853     if (nosh->printwhat[i] == NPT_ENERGY) {
00854         printEnergy(com, nosh, totEnergy, i);
00855         /* Print force */
00856     } else if (nosh->printwhat[i] == NPT_FORCE) {
00857         printForce(com, nosh, nforce, atomForce, i);
00858     } else if (nosh->printwhat[i] == NPT_ELECENERGY) {
00859         printElecEnergy(com, nosh, totEnergy, i);
00860     } else if (nosh->printwhat[i] == NPT_ELECFORCE) {
00861         printElecForce(com, nosh, nforce, atomForce, i);
00862     } else if (nosh->printwhat[i] == NPT_APOLENERGY) {
00863         printApolEnergy(nosh, i);
00864     } else if (nosh->printwhat[i] == NPT_APOLFORCE) {
00865         printApolForce(com, nosh, nforce, atomForce, i);
00866     } else {
00867         Vnm_tprint( 2, "Undefined PRINT keyword!\n");
00868         break;
00869     }
00870 }
00871 Vnm_tprint( 1, "-----\n");
00872
00873 /* ***** HANDLE LOGGING ***** */
00874
00875 if (outputformat == OUTPUT_FLAT) {
00876     Vnm_tprint(2, " Writing data to flat file %s...\n", output_path);
00877     writedataFlat(nosh, com, output_path, totEnergy, qfEnergy, qmEnergy,
00878                 dielEnergy, nenergy, atomEnergy, nforce, atomForce);
00879 }
00880
00881 /* Destroy energy arrays if they still exist */
00882
00883 for (i=0; i<nosh->ncalc; i++) {
00884     if (nenergy[i] > 0) Vmem_free(mem, nenergy[i], sizeof(double),
00885                               (void **)&(atomEnergy[i]));
00886 }
00887
00888 /* ***** GARBAGE COLLECTION ***** */
00889
00890 Vnm_tprint( 1, "CLEANING UP AND SHUTTING DOWN...\n");
00891 /* Clean up APBS structures */
00892 killForce(mem, nosh, nforce, atomForce);
00893 killEnergy();
00894 killMG(nosh, pbe, pmgp, pmg);
00895 #ifdef HAVE_MC_H
00896 killFE(nosh, pbe, fetk, gm);
00897 #endif
00898 killChargeMaps(nosh, chargeMap);
00899 killKappaMaps(nosh, kappaMap);
00900 killDielMaps(nosh, dielXMap, dielYMap, dielZMap);
00901 killMolecules(nosh, alist);
00902 NOsh_dtor(&nosh);
00903
00904 /* Memory statistics */
00905 bytesTotal = Vmem_bytesTotal();
00906 highWater = Vmem_highWaterTotal();
00907 Vnm_tprint( 1, "Final memory usage:  %4.3f MB total, %4.3f MB high water\n",
00908             (double) (bytesTotal)/(1024.*1024.),
00909             (double) (highWater)/(1024.*1024.));
00910
00911 /* Clean up MALOC structures */
00912 Vcom_dtor(&com);
00913 Vmem_dtor(&mem);
00914
00915 /* And now it's time to so "so long"... */
00916 Vnm_tprint(1, "\n\n");
00917 Vnm_tprint( 1, "Thanks for using APBS!\n\n");
00918

```



```

00919 #if defined(DEBUG_MAC_OSX_OCL)
00920     mets_(&mbeg, "Main Program CL");
00921 #endif
00922 #if defined(DEBUG_MAC_OSX_STANDARD)
00923     mets_(&mbeg, "Main Program Standard");
00924 #endif
00925
00926     /* This should be last */
00927     Vnm_tstop(APBS_TIMER_WALL_CLOCK, "APBS WALL CLOCK");
00928     Vnm_flush(1);
00929     Vnm_flush(2);
00930     Vcom_finalize();
00931
00932     fflush(NULL);
00933
00934     return 0;
00935
00936     ERROR1:
00937     Vcom_finalize();
00938     Vcom_dtor(&com);
00939     Vmem_dtor(&mem);
00940     return APBSRC;
00941 }

```

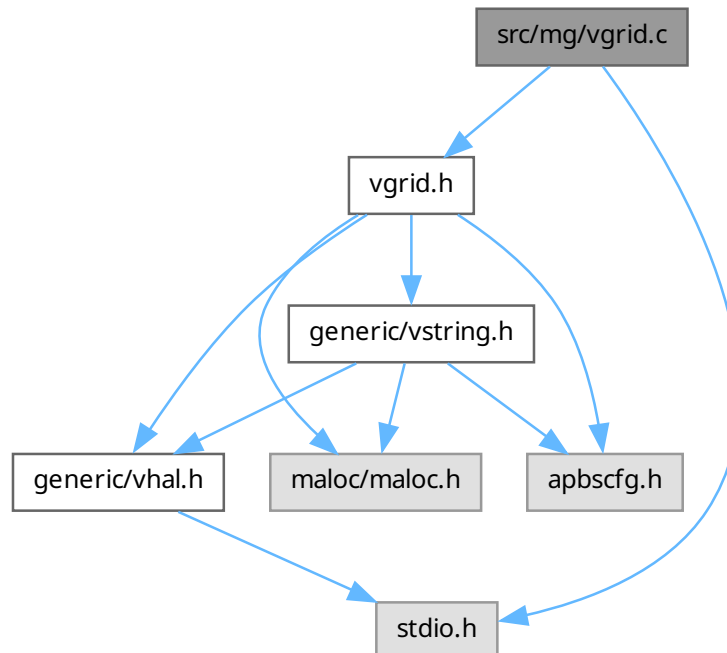
9.94 src/mg/vgrid.c File Reference

Class Vgrid methods.

```
#include "vgrid.h"
```

```
#include <stdio.h>
```

Include dependency graph for vgrid.c:



Macros

- #define **IJK**(i, j, k) (((k)*(nx)*(ny))+((j)*(nx))+(i))

Functions

- VPUBLIC unsigned long int **Vgrid_memChk** (**Vgrid** *thee)
Return the memory used by this structure (and its contents) in bytes.
- VPUBLIC **Vgrid** * **Vgrid_ctor** (int nx, int ny, int nz, double hx, double hy, double hzed, double xmin, double ymin, double zmin, double *data)
Construct Vgrid object with values obtained from Vpmg_readDX (for example)
- VPUBLIC int **Vgrid_ctor2** (**Vgrid** *thee, int nx, int ny, int nz, double hx, double hy, double hzed, double xmin, double ymin, double zmin, double *data)
Initialize Vgrid object with values obtained from Vpmg_readDX (for example)
- VPUBLIC void **Vgrid_dtor** (**Vgrid** **thee)
Object destructor.
- VPUBLIC void **Vgrid_dtor2** (**Vgrid** *thee)
FORTTRAN stub object destructor.
- VPUBLIC int **Vgrid_value** (**Vgrid** *thee, double pt[3], double *value)
Get potential value (from mesh or approximation) at a point.
- VPUBLIC int **Vgrid_curvature** (**Vgrid** *thee, double pt[3], int cflag, double *value)
Get second derivative values at a point.
- VPUBLIC int **Vgrid_gradient** (**Vgrid** *thee, double pt[3], double grad[3])
Get first derivative values at a point.
- VPUBLIC int **Vgrid_readGZ** (**Vgrid** *thee, const char *fname)
Read in OpenDX data in GZIP format.
- VPUBLIC int **Vgrid_readDX** (**Vgrid** *thee, const char *iodev, const char *iofmt, const char *thost, const char *fname)
Read in data in OpenDX grid format.
- VPUBLIC int **Vgrid_readDXBIN** (**Vgrid** *thee, const char *iodev, const char *iofmt, const char *thost, const char *fname)
Read in binary data in OpenDX grid format.
- VPUBLIC void **Vgrid_writeGZ** (**Vgrid** *thee, const char *iodev, const char *iofmt, const char *thost, const char *fname, char *title, double *pvec)
Write out OpenDX data in GZIP format.
- VPUBLIC void **Vgrid_writeDX** (**Vgrid** *thee, const char *iodev, const char *iofmt, const char *thost, const char *fname, char *title, double *pvec)
Write out the data in OpenDX grid format.
- VPUBLIC void **Vgrid_writeDXBIN** (**Vgrid** *thee, const char *iodev, const char *iofmt, const char *thost, const char *fname, char *title, double *pvec)
Write out the binary data in OpenDX grid format.
- VPUBLIC void **Vgrid_writeUHBD** (**Vgrid** *thee, const char *iodev, const char *iofmt, const char *thost, const char *fname, char *title, double *pvec)
Write out the data in UHBD grid format.
- VPUBLIC double **Vgrid_integrate** (**Vgrid** *thee)
Get the integral of the data.
- VPUBLIC double **Vgrid_normL1** (**Vgrid** *thee)
Get the L_1 norm of the data. This returns the integral:
- VPUBLIC double **Vgrid_normL2** (**Vgrid** *thee)

Get the L_2 norm of the data. This returns the integral:

- VPUBLIC double [Vgrid_seminormH1](#) ([Vgrid](#) *thee)

Get the H_1 semi-norm of the data. This returns the integral:

- VPUBLIC double [Vgrid_normH1](#) ([Vgrid](#) *thee)

Get the H_1 norm (or energy norm) of the data. This returns the integral:

- VPUBLIC double [Vgrid_normLinf](#) ([Vgrid](#) *thee)

Get the L_∞ norm of the data. This returns the integral:

Variables

- VPRIVATE char * [MCwhiteChars](#) = " =,;\t\n"
- VPRIVATE char * [MCcommChars](#) = "#%"
- VPRIVATE double [Vcompare](#)
- VPRIVATE char [Vprecision](#) [26]

9.94.1 Detailed Description

Class [Vgrid](#) methods.

Author

Nathan Baker

Version

\$Id\$

Attention

```
*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
* Nathan A. Baker (nathan.baker@pnnl.gov)
* Pacific Northwest National Laboratory
*
* Additional contributing authors listed in the code documentation.
*
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```

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*
*

```

Definition in file [vgrid.c](#).

9.94.2 Macro Definition Documentation

9.94.2.1 IJK

```

#define IJK(
    i,
    j,
    k ) ((k)*(nx)*(ny)) + ((j)*(nx)) + (i)

```

Definition at line 67 of file [vgrid.c](#).

9.94.3 Function Documentation

9.94.3.1 Vgrid_writeGZ()

```

VPUBLIC void Vgrid_writeGZ (
    Vgrid * thee,
    const char * iodev,
    const char * iofmt,
    const char * thost,
    const char * fname,
    char * title,
    double * pvec )

```

Write out OpenDX data in GZIP format.

Author

Dave Gohara

Parameters

<i>thee</i>	Object to hold new grid data
<i>iodev</i>	I/O device
<i>iofmt</i>	I/O format
<i>thost</i>	Remote host name
<i>fname</i>	File name
<i>title</i>	Data title
<i>pvec</i>	Masking vector (0 = not written)

Definition at line 1011 of file [vgrid.c](#).

9.94.4 Variable Documentation

9.94.4.1 MCcommChars

VPRIVATE char* MCcommChars = "#%"

Definition at line 78 of file [vgrid.c](#).

9.94.4.2 MCwhiteChars

VPRIVATE char* MCwhiteChars = " =,;\t\n"

Definition at line 77 of file [vgrid.c](#).

9.94.4.3 Vcompare

VPRIVATE double Vcompare

Definition at line 79 of file [vgrid.c](#).

9.94.4.4 Vprecision

VPRIVATE char Vprecision[26]

Definition at line 80 of file [vgrid.c](#).

9.95 vgrid.c

[Go to the documentation of this file.](#)

```

00001
00057 #include "vgrid.h"
00058 #include <stdio.h>
00059
00060 VEMBED(rcsid="$Id$")
00061
00062 #if !defined(VINLINE_VGRID)
00063     VPUBLIC unsigned long int Vgrid_memChk(Vgrid *thee) {
00064         return Vmem_bytes(thee->mem);
00065     }
00066 #endif
00067 #define IJK(i,j,k)  (((k)*(nx)*(ny))+((j)*(nx))+(i))
00068
00069 #if defined(_WIN32) && (_MSC_VER < 1800)
00070 #include <float.h>
00071 int isnan(double d)
00072 {
00073     return _isnan(d);
00074 }
00075 #endif
00076
00077 VPRIVATE char *MCwhiteChars = " =,;\t\n";
00078 VPRIVATE char *MCcommChars = "#%";
00079 VPRIVATE double Vcompare;
00080 VPRIVATE char Vprecision[26];
00081
00082 /* ////////////////////////////////////// */
00083 // Routine:  Vgrid_ctor
00084 // Author:   Nathan Baker
00086 VPUBLIC Vgrid* Vgrid_ctor(int nx,
00087                          int ny,
00088                          int nz,
00089                          double hx,
00090                          double hy,
00091                          double hzed,
00092                          double xmin,
00093                          double ymin,
00094                          double zmin,
00095                          double *data
00096                          ) {
00097
00098     Vgrid *thee = VNULL;
00099
00100     thee = (Vgrid*)Vmem_malloc(VNULL, 1, sizeof(Vgrid));
00101     VASSERT(thee != VNULL);

```

```

00102     VASSERT(Vgrid_ctor2(thee, nx, ny, nz, hx, hy, hzed,
00103                     xmin, ymin, zmin, data));
00104
00105     return thee;
00106 }
00107
00108 /* ////////////////////////////////////////
00109 // Routine:  Vgrid_ctor2
00110 // Author:   Nathan Baker
00112 VPUBLIC int Vgrid_ctor2(Vgrid *thee, int nx, int ny, int nz,
00113                     double hx, double hy, double hzed,
00114                     double xmin, double ymin, double zmin,
00115                     double *data) {
00116
00117     if (thee == VNULL) return 0;
00118     thee->nx = nx;
00119     thee->ny = ny;
00120     thee->nz = nz;
00121     thee->hx = hx;
00122     thee->hy = hy;
00123     thee->hzed = hzed;
00124     thee->xmin = xmin;
00125     thee->xmax = xmin + (nx-1)*hx;
00126     thee->ymin = ymin;
00127     thee->ymax = ymin + (ny-1)*hy;
00128     thee->zmin = zmin;
00129     thee->zmax = zmin + (nz-1)*hzed;
00130     if (data == VNULL) {
00131         thee->ctordata = 0;
00132         thee->readdata = 0;
00133     } else {
00134         thee->ctordata = 1;
00135         thee->readdata = 0;
00136         thee->data = data;
00137     }
00138
00139     thee->mem = Vmem_ctor("APBS:VGRID");
00140
00141     Vcompare = pow(10,-1*(VGRID_DIGITS - 2));
00142     sprintf(Vprecision,"%12.2de %12.2de %12.2de", VGRID_DIGITS,
00143           VGRID_DIGITS, VGRID_DIGITS);
00144
00145     return 1;
00146 }
00147
00148 /* ////////////////////////////////////////
00149 // Routine:  Vgrid_dtor
00150 // Author:   Nathan Baker
00152 VPUBLIC void Vgrid_dtor(Vgrid **thee) {
00153
00154     if ((*thee) != VNULL) {
00155         Vgrid_dtor2(*thee);
00156         Vmem_free(VNULL, 1, sizeof(Vgrid), (void **)thee);
00157         (*thee) = VNULL;
00158     }
00159 }
00160
00161 /* ////////////////////////////////////////
00162 // Routine:  Vgrid_dtor2
00163 // Author:   Nathan Baker
00165 VPUBLIC void Vgrid_dtor2(Vgrid *thee) {
00166
00167     if (thee->readdata) {
00168         Vmem_free(thee->mem, (thee->nx*thee->ny*thee->nz), sizeof(double),
00169             (void **)&(thee->data));
00170     }
00171     Vmem_dtor(&(thee->mem));
00172 }
00173 }
00174
00175 /* ////////////////////////////////////////
00176 // Routine:  Vgrid_value
00177 // Author:   Nathan Baker
00179 VPUBLIC int Vgrid_value(Vgrid *thee, double pt[3], double *value) {
00180
00181     int nx, ny, nz;
00182     size_t ihi, jhi, khi, ilo, jlo, klo;
00183     double hx, hy, hzed, xmin, ymin, zmin, ifloat, jfloat, kfloat;
00184     double xmax, ymax, zmax;
00185     double u, dx, dy, dz;
00186

```

```

00187     if (thee == VNULL) {
00188         Vnm_print(2, "Vgrid_value: Error -- got VNULL thee!\n");
00189         VASSERT(0);
00190     }
00191     if (!(thee->ctordata || thee->readdata)) {
00192         Vnm_print(2, "Vgrid_value: Error -- no data available!\n");
00193         VASSERT(0);
00194     }
00195
00196     nx = thee->nx;
00197     ny = thee->ny;
00198     nz = thee->nz;
00199     hx = thee->hx;
00200     hy = thee->hy;
00201     hzed = thee->hzed;
00202     xmin = thee->xmin;
00203     ymin = thee->ymin;
00204     zmin = thee->zmin;
00205     xmax = thee->xmax;
00206     ymax = thee->ymax;
00207     zmax = thee->zmax;
00208
00209     u = 0;
00210
00211     ifloat = (pt[0] - xmin)/hx;
00212     jfloat = (pt[1] - ymin)/hy;
00213     kfloat = (pt[2] - zmin)/hzed;
00214
00215     ihi = (int)ceil(ifloat);
00216     jhi = (int)ceil(jfloat);
00217     khi = (int)ceil(kfloat);
00218     ilo = (int)floor(ifloat);
00219     jlo = (int)floor(jfloat);
00220     klo = (int)floor(kfloat);
00221     if (VABS(pt[0] - xmin) < Vcompare) ilo = 0;
00222     if (VABS(pt[1] - ymin) < Vcompare) jlo = 0;
00223     if (VABS(pt[2] - zmin) < Vcompare) klo = 0;
00224     if (VABS(pt[0] - xmax) < Vcompare) ihi = nx-1;
00225     if (VABS(pt[1] - ymax) < Vcompare) jhi = ny-1;
00226     if (VABS(pt[2] - zmax) < Vcompare) khi = nz-1;
00227
00228     /* See if we're on the mesh */
00229     /*the condions starting with ilo>=0 seem unnecessary since they are of type size_t*/
00230     if ((ihi<nx) && (jhi<ny) && (khi<nz) /*&&
00231         (ilo>=0) && (jlo>=0) && (klo>=0)*/) {
00232
00233         dx = ifloat - (double)(ilo);
00234         dy = jfloat - (double)(jlo);
00235         dz = kfloat - (double)(klo);
00236         u = dx      *dy      *dz      *(thee->data[IJK(ihi, jhi, khi)])
00237           + dx      *(1.0-dy)*dz      *(thee->data[IJK(ihi, jlo, khi)])
00238           + dx      *dy      *(1.0-dz)*(thee->data[IJK(ihi, jhi, klo)])
00239           + dx      *(1.0-dy)*(1.0-dz)*(thee->data[IJK(ihi, jlo, klo)])
00240           + (1.0-dx)*dy      *dz      *(thee->data[IJK(ilo, jhi, khi)])
00241           + (1.0-dx)*(1.0-dy)*dz      *(thee->data[IJK(ilo, jlo, khi)])
00242           + (1.0-dx)*dy      *(1.0-dz)*(thee->data[IJK(ilo, jhi, klo)])
00243           + (1.0-dx)*(1.0-dy)*(1.0-dz)*(thee->data[IJK(ilo, jlo, klo)]);
00244
00245         *value = u;
00246
00247         if (isnan(u)) {
00248             Vnm_print(2, "Vgrid_value: Got NaN!\n");
00249             Vnm_print(2, "Vgrid_value: (x, y, z) = (%4.3f, %4.3f, %4.3f)\n",
00250                 pt[0], pt[1], pt[2]);
00251             Vnm_print(2, "Vgrid_value: (ihi, jhi, khi) = (%d, %d, %d)\n",
00252                 ihi, jhi, khi);
00253             Vnm_print(2, "Vgrid_value: (ilo, jlo, klo) = (%d, %d, %d)\n",
00254                 ilo, jlo, klo);
00255             Vnm_print(2, "Vgrid_value: (nx, ny, nz) = (%d, %d, %d)\n",
00256                 nx, ny, nz);
00257             Vnm_print(2, "Vgrid_value: (dx, dy, dz) = (%4.3f, %4.3f, %4.3f)\n",
00258                 dx, dy, dz);
00259             Vnm_print(2, "Vgrid_value: data[IJK(ihi, jhi, khi)] = %g\n",
00260                 thee->data[IJK(ihi, jhi, khi)]);
00261             Vnm_print(2, "Vgrid_value: data[IJK(ihi, jlo, khi)] = %g\n",
00262                 thee->data[IJK(ihi, jlo, khi)]);
00263             Vnm_print(2, "Vgrid_value: data[IJK(ihi, jhi, klo)] = %g\n",
00264                 thee->data[IJK(ihi, jhi, klo)]);
00265             Vnm_print(2, "Vgrid_value: data[IJK(ihi, jlo, klo)] = %g\n",
00266                 thee->data[IJK(ihi, jlo, klo)]);
00267             Vnm_print(2, "Vgrid_value: data[IJK(ilo, jhi, khi)] = %g\n",

```

```

00268         thee->data[IJK(ilo,jhi,khi)]);
00269     Vnm_print(2, "Vgrid_value:  data[IJK(ilo,jlo,khi)] = %g\n",
00270         thee->data[IJK(ilo,jlo,khi)]);
00271     Vnm_print(2, "Vgrid_value:  data[IJK(ilo,jhi,klo)] = %g\n",
00272         thee->data[IJK(ilo,jhi,klo)]);
00273     Vnm_print(2, "Vgrid_value:  data[IJK(ilo,jlo,klo)] = %g\n",
00274         thee->data[IJK(ilo,jlo,klo)]);
00275     }
00276     return 1;
00277 } else {
00278
00279     *value = 0;
00280     return 0;
00281 }
00282
00283 return 0;
00284 }
00285
00286 }
00287 }
00288
00289 /* ////////////////////////////////////////////////////////////////////
00290 // Routine:  Vgrid_curvature
00291 //
00292 // Notes:  cflag=0 ==> Reduced Maximal Curvature
00293 //         cflag=1 ==> Mean Curvature (Laplace)
00294 //         cflag=2 ==> Gauss Curvature
00295 //         cflag=3 ==> True Maximal Curvature
00296 //
00297 // Authors:  Stephen Bond and Nathan Baker
00299 VPUBLIC int Vgrid_curvature(Vgrid *thee, double pt[3], int cflag,
00300     double *value) {
00301
00302     double hx, hy, hzed, curv;
00303     double dxx, dyy, dzz;
00304     double uleft, umid, uright, testpt[3];
00305
00306     if (thee == VNULL) {
00307         Vnm_print(2, "Vgrid_curvature:  Error -- got VNULL thee!\n");
00308         VASSERT(0);
00309     }
00310     if (!(thee->ctordata || thee->readdata)) {
00311         Vnm_print(2, "Vgrid_curvature:  Error -- no data available!\n");
00312         VASSERT(0);
00313     }
00314
00315     hx = thee->hx;
00316     hy = thee->hy;
00317     hzed = thee->hzed;
00318
00319     curv = 0.0;
00320
00321     testpt[0] = pt[0];
00322     testpt[1] = pt[1];
00323     testpt[2] = pt[2];
00324
00325     /* Compute 2nd derivative in the x-direction */
00326     VJMPERR1(Vgrid_value( thee, testpt, &umid));
00327     testpt[0] = pt[0] - hx;
00328     VJMPERR1(Vgrid_value( thee, testpt, &uleft));
00329     testpt[0] = pt[0] + hx;
00330     VJMPERR1(Vgrid_value( thee, testpt, &uright));
00331     testpt[0] = pt[0];
00332
00333     dxx = (uright - 2*umid + uleft)/(hx*hx);
00334
00335     /* Compute 2nd derivative in the y-direction */
00336     VJMPERR1(Vgrid_value( thee, testpt, &umid));
00337     testpt[1] = pt[1] - hy;
00338     VJMPERR1(Vgrid_value( thee, testpt, &uleft));
00339     testpt[1] = pt[1] + hy;
00340     VJMPERR1(Vgrid_value( thee, testpt, &uright));
00341     testpt[1] = pt[1];
00342
00343     dyy = (uright - 2*umid + uleft)/(hy*hy);
00344
00345     /* Compute 2nd derivative in the z-direction */
00346     VJMPERR1(Vgrid_value( thee, testpt, &umid));
00347     testpt[2] = pt[2] - hzed;
00348     VJMPERR1(Vgrid_value( thee, testpt, &uleft));
00349     testpt[2] = pt[2] + hzed;

```



```

00350     VJMPERR1(Vgrid_value( thee, testpt, &uright));
00351
00352     dzz = (uright - 2*umid + uleft)/(hzd*hzd);
00353
00354
00355     if ( cflag == 0 ) {
00356         curv = fabs(dxx);
00357         curv = ( curv > fabs(dyy) ) ? curv : fabs(dyy);
00358         curv = ( curv > fabs(dzz) ) ? curv : fabs(dzz);
00359     } else if ( cflag == 1 ) {
00360         curv = (dxx + dyy + dzz)/3.0;
00361     } else {
00362         Vnm_print(2, "Vgrid_curvature: support for cflag = %d not available!\n", cflag);
00363         VASSERT( 0 ); /* Feature Not Coded Yet! */
00364     }
00365
00366     *value = curv;
00367     return 1;
00368
00369     VERROR1:
00370         return 0;
00371 }
00372
00373
00374 /* ////////////////////////////////////////
00375 // Routine: Vgrid_gradient
00376 //
00377 // Authors: Nathan Baker and Stephen Bond
00379 VPUBLIC int Vgrid_gradient(Vgrid *thee, double pt[3], double grad[3]) {
00380
00381     double hx, hy, hzed;
00382     double uleft, umid, uright, testpt[3];
00383     int haveleft, haveright;
00384
00385     if (thee == VNULL) {
00386         Vnm_print(2, "Vgrid_gradient: Error -- got VNULL thee!\n");
00387         VASSERT(0);
00388     }
00389     if (!(thee->ctordata || thee->readdata)) {
00390         Vnm_print(2, "Vgrid_gradient: Error -- no data available!\n");
00391         VASSERT(0);
00392     }
00393
00394     hx = thee->hx;
00395     hy = thee->hy;
00396     hzed = thee->hzd;
00397
00398     /* Compute derivative in the x-direction */
00399     testpt[0] = pt[0];
00400     testpt[1] = pt[1];
00401     testpt[2] = pt[2];
00402     VJMPERR1( Vgrid_value( thee, testpt, &umid));
00403     testpt[0] = pt[0] - hx;
00404     if (Vgrid_value( thee, testpt, &uleft)) haveleft = 1;
00405     else haveleft = 0;
00406     testpt[0] = pt[0] + hx;
00407     if (Vgrid_value( thee, testpt, &uright)) haveright = 1;
00408     else haveright = 0;
00409     if (haveright && haveleft) grad[0] = (uright - uleft)/(2*hx);
00410     else if (haveright) grad[0] = (uright - umid)/hx;
00411     else if (haveleft) grad[0] = (umid - uleft)/hx;
00412     else VJMPERR1(0);
00413
00414     /* Compute derivative in the y-direction */
00415     testpt[0] = pt[0];
00416     testpt[1] = pt[1];
00417     testpt[2] = pt[2];
00418     VJMPERR1(Vgrid_value(thee, testpt, &umid));
00419     testpt[1] = pt[1] - hy;
00420     if (Vgrid_value( thee, testpt, &uleft)) haveleft = 1;
00421     else haveleft = 0;
00422     testpt[1] = pt[1] + hy;
00423     if (Vgrid_value( thee, testpt, &uright)) haveright = 1;
00424     else haveright = 0;
00425     if (haveright && haveleft) grad[1] = (uright - uleft)/(2*hy);
00426     else if (haveright) grad[1] = (uright - umid)/hy;
00427     else if (haveleft) grad[1] = (umid - uleft)/hy;
00428     else VJMPERR1(0);
00429
00430     /* Compute derivative in the z-direction */
00431     testpt[0] = pt[0];

```

```

00432     testpt[1] = pt[1];
00433     testpt[2] = pt[2];
00434     VJMPERR1(Vgrid_value(thee, testpt, &umid));
00435     testpt[2] = pt[2] - hzed;
00436     if (Vgrid_value(thee, testpt, &uleft)) haveleft = 1;
00437     else haveleft = 0;
00438     testpt[2] = pt[2] + hzed;
00439     if (Vgrid_value(thee, testpt, &uright)) haveright = 1;
00440     else haveright = 0;
00441     if (haveright && haveleft) grad[2] = (uright - uleft)/(2*hzed);
00442     else if (haveright) grad[2] = (uright - umid)/hzed;
00443     else if (haveleft) grad[2] = (umid - uleft)/hzed;
00444     else VJMPERR1(0);
00445
00446     return 1;
00447
00448     VERROR1:
00449     return 0;
00450
00451 }
00452
00453 /* ////////////////////////////////////////
00454 // Routine:  Vgrid_readGZ
00455 //
00456 // Author:   David Gohara
00457 #ifndef HAVE_ZLIB
00458 #define off_t long
00459 #include "zlib.h"
00460 #endif
00461 #endif
00462 VPUBLIC int Vgrid_readGZ(Vgrid *thee, const char *fname) {
00463
00464 #ifndef HAVE_ZLIB
00465     size_t i, j, k, u;
00466     size_t len; // Temporary counter variable for loop conditionals
00467     size_t header, incr;
00468     double *temp;
00469     double dtmpl, dtmp2, dtmp3;
00470     gzFile infile;
00471     char line[VMAX_ARGLEN];
00472
00473     header = 0;
00474
00475     /* Check to see if the existing data is null and, if not, clear it out */
00476     if (thee->data != VNULL) {
00477         Vnm_print(1, "%s:  destroying existing data!\n", __func__);
00478         Vmem_free(thee->mem, thee->nx * thee->ny * thee->nz, sizeof(double),
00479                 (void **)&(thee->data));
00480     }
00481
00482     thee->readdata = 1;
00483     thee->ctordata = 0;
00484
00485     infile = gzopen(fname, "rb");
00486     if (infile == Z_NULL) {
00487         Vnm_print(2, "%s:  Problem opening compressed file %s\n", __func__, fname);
00488         return VRC_FAILURE;
00489     }
00490
00491     thee->hx = 0.0;
00492     thee->hy = 0.0;
00493     thee->hzed = 0.0;
00494
00495     //read data here
00496     while (header < 7) {
00497         if (gzgets(infile, line, VMAX_ARGLEN) == Z_NULL){
00498             return VRC_FAILURE;
00499         }
00500
00501         // Skip comments and newlines
00502         if (strncmp(line, "#", 1) == 0) continue;
00503         if (line[0] == '\n') continue;
00504
00505         switch (header) {
00506             case 0:
00507                 sscanf(line, "object 1 class gridpositions counts %d %d %d",
00508                        &(thee->nx), &(thee->ny), &(thee->nz));
00509                 break;
00510             case 1:
00511                 sscanf(line, "origin %lf %lf %lf",
00512                        &(thee->xmin), &(thee->ymin), &(thee->zmin));
00513                 break;

```

```

00514         case 2:
00515         case 3:
00516         case 4:
00517             sscanf(line, "delta %lf %lf %lf", &dtmpl, &dtmp2, &dtmp3);
00518             thee->hx += dtmpl;
00519             thee->hy += dtmp2;
00520             thee->hz += dtmp3;
00521             break;
00522         default:
00523             break;
00524     }
00525
00526     header++;
00527 }
00528
00529 /* Allocate space for the data */
00530 Vnm_print(0, "%s: allocating %d x %d x %d doubles for storage\n",
00531     __func__, thee->nx, thee->ny, thee->nz);
00532 len = thee->nx * thee->ny * thee->nz;
00533
00534 thee->data = VNULL;
00535 thee->data = Vmem_malloc(thee->mem, len, sizeof(double));
00536 if (thee->data == VNULL) {
00537     Vnm_print(2, "%s: Unable to allocate space for data!\n", __func__);
00538     return 0;
00539 }
00540
00541 /* Allocate a temporary buffer to store the compressed
00542  * data into (column major order). Add 2 to ensure the buffer is
00543  * big enough to take extra data on the final read loop.
00544  */
00545 temp = (double *)malloc(len * (2 * sizeof(double)));
00546
00547 for (i = 0; i < len; i += 3) {
00548     memset(&line, 0, sizeof(line));
00549     gzgets(infile, line, VMAX_ARGLEN);
00550     sscanf(line, "%lf %lf %lf", &temp[i], &temp[i+1], &temp[i+2]);
00551 }
00552
00553 /* Now move the data to row major order */
00554 incr = 0;
00555 for (i=0; i<thee->nx; i++) {
00556     for (j=0; j<thee->ny; j++) {
00557         for (k=0; k<thee->nz; k++) {
00558             u = k*(thee->nx)*(thee->ny)+j*(thee->nx)+i;
00559             (thee->data)[u] = temp[incr++];
00560         }
00561     }
00562 }
00563
00564 /* calculate grid maxima */
00565 thee->xmax = thee->xmin + (thee->nx-1)*thee->hx;
00566 thee->ymax = thee->ymin + (thee->ny-1)*thee->hy;
00567 thee->zmax = thee->zmin + (thee->nz-1)*thee->hz;
00568
00569 /* Close off the socket */
00570 gzclose(infile);
00571 free(temp);
00572 #else
00573
00574 Vnm_print(0, "WARNING\n");
00575 Vnm_print(0, "Vgrid_readGZ:  gzip read/write support is disabled in this build\n");
00576 Vnm_print(0, "Vgrid_readGZ:  configure and compile without the --disable-zlib flag.\n");
00577 Vnm_print(0, "WARNING\n");
00578 #endif
00579 return VRC_SUCCESS;
00580 }
00581
00586 VPUBLIC int Vgrid_readDX(Vgrid *thee,
00587     const char *iodev,
00588     const char *iofmt,
00589     const char *thost,
00590     const char *fname
00591 ) {
00592
00593     size_t i, j, k, itmp, u;
00594     double dtmp;
00595     char tok[VMAX_BUFSIZE];
00596     Vio *sock;
00597
00598     /* Check to see if the existing data is null and, if not, clear it out */

```

```

00599     if (thee->data != VNULL) {
00600         Vnm_print(1, "Vgrid_readDX: destroying existing data!\n");
00601         Vmem_free(thee->mem, (thee->nx*thee->ny*thee->nz), sizeof(double),
00602             (void **)&(thee->data)); }
00603     thee->readdata = 1;
00604     thee->ctordata = 0;
00605
00606     /* Set up the virtual socket */
00607     sock = Vio_ctor(iodev, iofmt, thost, fname, "r");
00608     if (sock == VNULL) {
00609         Vnm_print(2, "Vgrid_readDX: Problem opening virtual socket %s\n",
00610             fname);
00611         return 0;
00612     }
00613     if (Vio_accept(sock, 0) < 0) {
00614         Vnm_print(2, "Vgrid_readDX: Problem accepting virtual socket %s\n",
00615             fname);
00616         return 0;
00617     }
00618
00619     Vio_setWhiteChars(sock, MCwhiteChars);
00620     Vio_setCommChars(sock, MCcommChars);
00621
00622     /* Read in the DX regular positions */
00623     /* Get "object" */
00624     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00625     VJMPERR1(!strcmp(tok, "object"));
00626     /* Get "l" */
00627     VJMPERR2(1 == Vio_scanf(sock, "%d", &itmp));
00628     /* Get "class" */
00629     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00630     VJMPERR1(!strcmp(tok, "class"));
00631     /* Get "gridpositions" */
00632     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00633     VJMPERR1(!strcmp(tok, "gridpositions"));
00634     /* Get "counts" */
00635     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00636     VJMPERR1(!strcmp(tok, "counts"));
00637     /* Get nx */
00638     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00639     VJMPERR1(1 == sscanf(tok, "%d", &(thee->nx)));
00640     /* Get ny */
00641     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00642     VJMPERR1(1 == sscanf(tok, "%d", &(thee->ny)));
00643     /* Get nz */
00644     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00645     VJMPERR1(1 == sscanf(tok, "%d", &(thee->nz)));
00646     Vnm_print(0, "Vgrid_readDX: Grid dimensions %d x %d x %d grid\n",
00647         thee->nx, thee->ny, thee->nz);
00648     /* Get "origin" */
00649     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00650     VJMPERR1(!strcmp(tok, "origin"));
00651     /* Get xmin */
00652     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00653     VJMPERR1(1 == sscanf(tok, "%lf", &(thee->xmin)));
00654     /* Get ymin */
00655     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00656     VJMPERR1(1 == sscanf(tok, "%lf", &(thee->ymin)));
00657     /* Get zmin */
00658     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00659     VJMPERR1(1 == sscanf(tok, "%lf", &(thee->zmin)));
00660     Vnm_print(0, "Vgrid_readDX: Grid origin = (%g, %g, %g)\n",
00661         thee->xmin, thee->ymin, thee->zmin);
00662     /* Get "delta" */
00663     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00664     VJMPERR1(!strcmp(tok, "delta"));
00665     /* Get hx */
00666     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00667     VJMPERR1(1 == sscanf(tok, "%lf", &(thee->hx)));
00668     /* Get 0.0 */
00669     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00670     VJMPERR1(1 == sscanf(tok, "%lf", &dtmp));
00671     VJMPERR1(dtmp == 0.0);
00672     /* Get 0.0 */
00673     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00674     VJMPERR1(1 == sscanf(tok, "%lf", &dtmp));
00675     VJMPERR1(dtmp == 0.0);
00676     /* Get "delta" */
00677     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00678     VJMPERR1(!strcmp(tok, "delta"));
00679     /* Get 0.0 */

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```

00680     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00681     VJMPERR1(1 == sscanf(tok, "%lf", &dtmp));
00682     VJMPERR1(dtmp == 0.0);
00683     /* Get hy */
00684     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00685     VJMPERR1(1 == sscanf(tok, "%lf", &(thee->hy)));
00686     /* Get 0.0 */
00687     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00688     VJMPERR1(1 == sscanf(tok, "%lf", &dtmp));
00689     VJMPERR1(dtmp == 0.0);
00690     /* Get "delta" */
00691     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00692     VJMPERR1(!strcmp(tok, "delta"));
00693     /* Get 0.0 */
00694     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00695     VJMPERR1(1 == sscanf(tok, "%lf", &dtmp));
00696     VJMPERR1(dtmp == 0.0);
00697     /* Get 0.0 */
00698     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00699     VJMPERR1(1 == sscanf(tok, "%lf", &dtmp));
00700     VJMPERR1(dtmp == 0.0);
00701     /* Get hz */
00702     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00703     VJMPERR1(1 == sscanf(tok, "%lf", &(thee->hz)));
00704     Vnm_print(0, "Vgrid_readDX: Grid spacings = (%g, %g, %g)\n",
00705               thee->hx, thee->hy, thee->hz);
00706     /* Get "object" */
00707     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00708     VJMPERR1(!strcmp(tok, "object"));
00709     /* Get "2" */
00710     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00711     /* Get "class" */
00712     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00713     VJMPERR1(!strcmp(tok, "class"));
00714     /* Get "gridconnections" */
00715     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00716     VJMPERR1(!strcmp(tok, "gridconnections"));
00717     /* Get "counts" */
00718     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00719     VJMPERR1(!strcmp(tok, "counts"));
00720     /* Get the dimensions again */
00721     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00722     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00723     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00724     /* Get "object" */
00725     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00726     VJMPERR1(!strcmp(tok, "object"));
00727     /* Get # */
00728     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00729     /* Get "class" */
00730     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00731     VJMPERR1(!strcmp(tok, "class"));
00732     /* Get "array" */
00733     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00734     VJMPERR1(!strcmp(tok, "array"));
00735     /* Get "type" */
00736     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00737     VJMPERR1(!strcmp(tok, "type"));
00738     /* Get "double" */
00739     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00740     VJMPERR1(!strcmp(tok, "double"));
00741     /* Get "rank" */
00742     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00743     VJMPERR1(!strcmp(tok, "rank"));
00744     /* Get # */
00745     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00746     /* Get "items" */
00747     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00748     VJMPERR1(!strcmp(tok, "items"));
00749     /* Get # */
00750     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00751     VJMPERR1(1 == sscanf(tok, "%lu", &itmp));
00752     u = (size_t)thee->nx * thee->ny * thee->nz;
00753     VJMPERR1(u == itmp);
00754     /* Get "data" */
00755     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00756     VJMPERR1(!strcmp(tok, "data"));
00757     /* Get "follows" */
00758     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00759     VJMPERR1(!strcmp(tok, "follows"));
00760

```

```

00761      /* Allocate space for the data */
00762      Vnm_print(0, "Vgrid_readDX: allocating %d x %d x %d doubles for storage\n",
00763        thee->nx, thee->ny, thee->nz);
00764      thee->data = VNULL;
00765      thee->data = (double*)Vmem_malloc(thee->mem, u, sizeof(double));
00766      if (thee->data == VNULL) {
00767          Vnm_print(2, "Vgrid_readDX: Unable to allocate space for data!\n");
00768          return 0;
00769      }
00770
00771      for (i=0; i<thee->nx; i++) {
00772          for (j=0; j<thee->ny; j++) {
00773              for (k=0; k<thee->nz; k++) {
00774                  u = k*(thee->nx)*(thee->ny)+j*(thee->nx)+i;
00775                  VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00776                  VJMPERR1(1 == sscanf(tok, "%lf", &dtmp));
00777                  (thee->data)[u] = dtmp;
00778              }
00779          }
00780      }
00781
00782      /* calculate grid maxima */
00783      thee->xmax = thee->xmin + (thee->nx-1)*thee->hx;
00784      thee->ymin = thee->ymin + (thee->ny-1)*thee->hy;
00785      thee->zmax = thee->zmin + (thee->nz-1)*thee->hz;
00786
00787      /* Close off the socket */
00788      Vio_acceptFree(sock);
00789      Vio_dtor(&sock);
00790
00791      return 1;
00792
00793  ERROR1:
00794      Vio_dtor(&sock);
00795      Vnm_print(2, "Vgrid_readDX: Format problem with input file < %s>\n",
00796        fname);
00797      return 0;
00798
00799  ERROR2:
00800      Vio_dtor(&sock);
00801      Vnm_print(2, "Vgrid_readDX: I/O problem with input file < %s>\n",
00802        fname);
00803      return 0;
00804 }
00805
00810 VPUBLIC int Vgrid_readDXBIN(Vgrid *thee, const char *iodev, const char *iofmt,
00811   const char *thost, const char *fname) {
00812
00813     size_t i, j, k, itmp, u;
00814     double dtmp, dtmp2;
00815     char tok[VMAX_BUFSIZE];
00816     int isBinary = 0;
00817     //Vio *sock;
00818
00819     /* Check to see if the existing data is null and, if not, clear it out */
00820     if (thee->data != VNULL) {
00821         Vnm_print(1, "Vgrid_readDXBIN: destroying existing data!\n");
00822         Vmem_free(thee->mem, (thee->nx*thee->ny*thee->nz), sizeof(double),
00823           (void **)&(thee->data)); }
00824     thee->readdata = 1;
00825     thee->ctordata = 0;
00826
00827     /*Open file fd for binary reading*/
00828     FILE *fd = fopen(fname, "rb");
00829     if (fd == NULL){
00830         printf("Vgrid_readDXBIN: Problem opening file %s\n", fname);
00831         fclose(fd);
00832         return 0;
00833     }
00834
00835     /* Set up the virtual socket */
00836     // sock = Vio_ctor(iodev, iofmt, thost, fname, "r");
00837     // if (sock == VNULL) {
00838     //     Vnm_print(2, "Vgrid_readDX: Problem opening virtual socket %s\n",
00839     //       fname);
00840     //     return 0;
00841     // }
00842     // if (Vio_accept(sock, 0) < 0) {
00843     //     Vnm_print(2, "Vgrid_readDX: Problem accepting virtual socket %s\n",
00844     //       fname);
00845     //     return 0;

```

```

00846 //      }
00847 //
00848 //      Vio_setWhiteChars(sock, MCwhiteChars);
00849 //      Vio_setCommChars(sock, MCcommChars);
00850
00851 //skip comments
00852 do{
00853     fgets(tok, VMAX_BUFSIZE, fd);
00854 }
00855 while(tok[0]!='#');
00856
00857 //get counts
00858 if(sscanf(tok,"object 1 class gridpositions counts %i %i %i\n",&(thee->nx),&(thee->ny),&(thee->nz))!= 3){
00859     printf("Vgrid_readDXBIN: Failed to read dimensions.\n");
00860     fclose(fd);
00861     return 0;
00862 }
00863 printf("Vgrid_readDXBIN: Grid dimensions %d x %d x %d grid\n",thee->nx, thee->ny, thee->nz);
00864
00865     /* Read in the DX regular positions */
00866
00867 /* Get "object" */
00868 //     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00869 //     VJMPERR1(!strcmp(tok, "object"));
00870 //     /* Get "1" */
00871 //     VJMPERR2(1 == Vio_scanf(sock, "%d", &itmp));
00872 //     /* Get "class" */
00873 //     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00874 //     VJMPERR1(!strcmp(tok, "class"));
00875 //     /* Get "gridpositions" */
00876 //     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00877 //     VJMPERR1(!strcmp(tok, "gridpositions"));
00878 //     /* Get "counts" */
00879 //     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00880 //     VJMPERR1(!strcmp(tok, "counts"));
00881 //     /* Get nx */
00882 //     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00883 //     VJMPERR1(1 == sscanf(tok, "%d", &(thee->nx)));
00884 //     /* Get ny */
00885 //     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00886 //     VJMPERR1(1 == sscanf(tok, "%d", &(thee->ny)));
00887 //     /* Get nz */
00888 //     VJMPERR2(1 == Vio_scanf(sock, "%s", tok));
00889 //     VJMPERR1(1 == sscanf(tok, "%d", &(thee->nz)));
00890 //     Vnm_print(0, "Vgrid_readDX: Grid dimensions %d x %d x %d grid\n",
00891 //         thee->nx, thee->ny, thee->nz);
00892
00893 if(fgets(tok,VMAX_BUFSIZE, fd) == NULL){
00894     printf("Vgrid_readDXBIN: unexpected end of file.\n");
00895     fclose(fd);
00896     return 0;
00897 }
00898 if(sscanf(tok,"origin %lf %lf %lf",&(thee->xmin),&(thee->ymin),&(thee->zmin))!=3){
00899     printf("Vgrid_readDXBIN: Failed to read origin cell data.\n");
00900     fclose(fd);
00901     return 0;
00902 }
00903 printf("Vgrid_readDXBIN: Grid origin = (%g %g %g)\n",thee->xmin, thee->ymin, thee->zmin);
00904
00905 //get Delta x
00906 if(fgets(tok,VMAX_BUFSIZE, fd) == NULL){
00907     printf("Vgrid_readDXBIN: unexpected end of file.\n");
00908     fclose(fd);
00909     return 0;
00910 }
00911 if(sscanf(tok,"delta %lf %lf %lf",&(thee->hx),&dtmp,&dtmp2)!=3){
00912     printf("Vgrid_readDXBIN: Failed to read delta x data.\n");
00913     fclose(fd);
00914     return 0;
00915 }
00916 //get Delta y
00917 if(fgets(tok,VMAX_BUFSIZE, fd) == NULL){
00918     printf("Vgrid_readDXBIN: Unexpected end of file\n");
00919     fclose(fd);
00920     return 0;
00921 }
00922 if(sscanf(tok,"delta %lf %lf %lf",&dtmp,&(thee->hy),&dtmp2)!=3){
00923     printf("Vgrid_readDXBIN: Failed to read delta y data.\n");
00924     fclose(fd);
00925     return 0;
00926 }

```

```

00927 //get Delta z
00928 if(fgets(tok,VMAX_BUFSIZE, fd) == NULL){
00929     printf("Vgrid_readDXBIN: Unexpected end of file.\n");
00930     fclose(fd);
00931     return 0;
00932 }
00933 if(sscanf(tok,"delta %lf %lf %lf",&dtmp,&dtmp2,&(thee->hzd))!=3){
00934     printf("Vgrid_readDXBIN: Failed to read delta z data.\n");
00935     fclose(fd);
00936     return 0;
00937 }
00938 printf("Vgrid_readDXBIN: Grid spacings = (%g, %g, %g)\n",thee->hx, thee->hy, thee->hzd);
00939
00940 //skip a line
00941 if(fgets(tok,VMAX_BUFSIZE, fd) == NULL){
00942     printf("Vgrid_readDXBIN: Unexpected end of file.\n");
00943     fclose(fd);
00944     return 0;
00945 }
00946
00947 //scan the buffer for the word binary
00948 if(fgets(tok,VMAX_BUFSIZE, fd) == NULL){
00949     printf("Vgrid_readDXBIN: Unexpected end of file.\n");
00950     fclose(fd);
00951     return 0;
00952 }
00953 if(strstr(tok,"binary")){
00954     isBinary = 1;
00955 }
00956 else{
00957     printf("Vgrid_readDXBIN: Binary tag not found. Will continue to try to read binary data.");
00958 }
00959
00960 u = (size_t)thee->nx * thee->ny * thee->nz;
00961 int tot = thee->nx * thee->ny * thee->nz;
00962
00963 /*Allocate space for the data*/
00964 printf("Vgrid_readDXBIN: allocating %d x %d x %d doubled for storage\n", thee->nx, thee->ny, thee->nz);
00965 thee->data = NULL;
00966 thee->data = (double *)malloc(tot*sizeof(double));
00967
00968 if(thee->data == NULL){
00969     printf("Vgrid_readDXBIN: Unable to allocate space for data!\n");
00970     fclose(fd);
00971     return 0;
00972 }
00973
00974 int counter = 0, r;
00975
00976 for (i=0; i<thee->nx; i++) {
00977     for (j=0; j<thee->ny; j++) {
00978         for (k=0; k<thee->nz; k++) {
00979             u = k*(thee->nx)*(thee->ny)+j*(thee->nx)+i;
00980             r = fread(&dtmp,sizeof(double),1,fd);
00981             (thee->data)[u] = dtmp;
00982             if(r!= 1){
00983                 printf("Vgrid_readDXBIN: Failed to read doubles.\n");
00984                 return 0;
00985             }
00986             counter++;
00987         }
00988     }
00989 }
00990
00991 if(counter!=tot){
00992     printf("Vgrid_readDXBIN: Read double = %d not equal to items = %d\n",counter, tot);
00993 }
00994
00995 /* calculate grid maxima */
00996 thee->xmax = thee->xmin + (thee->nx-1)*thee->hx;
00997 thee->ymax = thee->ymin + (thee->ny-1)*thee->hy;
00998 thee->zmax = thee->zmin + (thee->nz-1)*thee->hzd;
00999
01000 fclose(fd);
01001
01002 return 1;
01003 }
01004
01005
01006 /* ////////////////////////////////////////
01007 // Routine: Vgrid_writeGZ

```



```

01008 //
01009 // Author:   Nathan Baker
01011 VPUBLIC void Vgrid_writeGZ(Vgrid *thee, const char *iodev, const char *iofmt,
01012                          const char *thost, const char *fname, char *title, double *pvec) {
01013
01014 #ifdef HAVE_ZLIB
01015     double xmin, ymin, zmin, hx, hy, hzed;
01016
01017     int nx, ny, nz, nxPART, nyPART, nzPART;
01018     int usepart, gotit;
01019     size_t icol, i, j, k, u;
01020     double x, y, z, xminPART, yminPART, zminPART;
01021
01022     size_t txyz;
01023     double txmin, tymin, tzmin;
01024
01025     char header[8196];
01026     char footer[8196];
01027     char line[80];
01028     char newline[] = "\n";
01029     gzFile outfile;
01030     char precFormat[VMAX_BUFSIZE];
01031
01032     if (thee == VNULL) {
01033         Vnm_print(2, "Vgrid_writeGZ: Error -- got VNULL thee!\n");
01034         VASSERT(0);
01035     }
01036     if (!(thee->ctordata || thee->readdata)) {
01037         Vnm_print(2, "Vgrid_writeGZ: Error -- no data available!\n");
01038         VASSERT(0);
01039     }
01040
01041     hx = thee->hx;
01042     hy = thee->hy;
01043     hzed = thee->hzed;
01044     nx = thee->nx;
01045     ny = thee->ny;
01046     nz = thee->nz;
01047     xmin = thee->xmin;
01048     ymin = thee->ymin;
01049     zmin = thee->zmin;
01050
01051     if (pvec == VNULL) usepart = 0;
01052     else usepart = 1;
01053
01054     /* Set up the virtual socket */
01055     Vnm_print(0, "Vgrid_writeGZ: Opening file...\n");
01056     outfile = gzopen(fname, "wb");
01057
01058     if (usepart) {
01059         /* Get the lower corner and number of grid points for the local
01060          * partition */
01061         xminPART = VLARGE;
01062         yminPART = VLARGE;
01063         zminPART = VLARGE;
01064         nxPART = 0;
01065         nyPART = 0;
01066         nzPART = 0;
01067         /* First, search for the lower corner */
01068         for (k=0; k<nz; k++) {
01069             z = k*hzed + zmin;
01070             for (j=0; j<ny; j++) {
01071                 y = j*hy + ymin;
01072                 for (i=0; i<nx; i++) {
01073                     x = i*hx + xmin;
01074                     if (pvec[IJK(i,j,k)] > 0.0) {
01075                         if (x < xminPART) xminPART = x;
01076                         if (y < yminPART) yminPART = y;
01077                         if (z < zminPART) zminPART = z;
01078                     }
01079                 }
01080             }
01081         }
01082         /* Now search for the number of grid points in the z direction */
01083         for (k=0; k<nz; k++) {
01084             gotit = 0;
01085             for (j=0; j<ny; j++) {
01086                 for (i=0; i<nx; i++) {
01087                     if (pvec[IJK(i,j,k)] > 0.0) {
01088                         gotit = 1;
01089                         break;

```

```

01090         }
01091     }
01092     if (gotit) break;
01093 }
01094 if (gotit) nzPART++;
01095 }
01096 /* Now search for the number of grid points in the y direction */
01097 for (j=0; j<ny; j++) {
01098     gotit = 0;
01099     for (k=0; k<nz; k++) {
01100         for (i=0; i<nx; i++) {
01101             if (pvec[IJK(i,j,k)] > 0.0) {
01102                 gotit = 1;
01103                 break;
01104             }
01105         }
01106         if (gotit) break;
01107     }
01108     if (gotit) nyPART++;
01109 }
01110 /* Now search for the number of grid points in the x direction */
01111 for (i=0; i<nx; i++) {
01112     gotit = 0;
01113     for (k=0; k<nz; k++) {
01114         for (j=0; j<ny; j++) {
01115             if (pvec[IJK(i,j,k)] > 0.0) {
01116                 gotit = 1;
01117                 break;
01118             }
01119         }
01120         if (gotit) break;
01121     }
01122     if (gotit) nxPART++;
01123 }
01124
01125 if ((nxPART != nx) || (nyPART != ny) || (nzPART != nz)) {
01126     Vnm_print(0, "Vgrid_writeGZ: printing only subset of domain\n");
01127 }
01128
01129 txyz = (nxPART*nyPART*nzPART);
01130 txmin = xminPART;
01131 tymin = yminPART;
01132 tzmin = zminPART;
01133
01134 }else {
01135
01136     txyz = (nx*ny*nz);
01137     txmin = xmin;
01138     tymin = ymin;
01139     tzmin = zmin;
01140
01141 }
01142
01143 /* Write off the title (if we're not XDR) */
01144 sprintf(header,
01145     "# Data from %s\n" \
01146     "# \n" \
01147     "# %s\n" \
01148     "# \n" \
01149     "object 1 class gridpositions counts %i %i %i\n" \
01150     "origin %12.6e %12.6e %12.6e\n" \
01151     "delta %12.6e 0.000000e+00 0.000000e+00\n" \
01152     "delta 0.000000e+00 %12.6e 0.000000e+00\n" \
01153     "delta 0.000000e+00 0.000000e+00 %12.6e\n" \
01154     "object 2 class gridconnections counts %i %i %i\n" \
01155     "object 3 class array type double rank 0 items %lu data follows\n",
01156     PACKAGE_STRING,title,nx,ny,nz,txmin,tymin,tzmin,
01157     hx,hy,hzed,nx,ny,nz,txyz);
01158 gzwrite(outfile, header, strlen(header)*sizeof(char));
01159
01160 /* Now write the data */
01161 icol = 0;
01162 for (i=0; i<nx; i++) {
01163     for (j=0; j<ny; j++) {
01164         for (k=0; k<nz; k++) {
01165             u = k*(nx)*(ny)+j*(nx)+i;
01166             if (pvec[u] > 0.0) {
01167                 sprintf(line, "%12.6e ", thee->data[u]);
01168                 gzwrite(outfile, line, strlen(line)*sizeof(char));
01169                 icol++;
01170                 if (icol == 3) {

```

```

01171             icol = 0;
01172             gzwrite(outfile, newline, strlen(newline)*sizeof(char));
01173         }
01174     }
01175 }
01176 }
01177 }
01178 if(icol < 3){
01179     char newline[] = "\n";
01180     gzwrite(outfile, newline, strlen(newline)*sizeof(char));
01181 }
01182
01183 /* Create the field */
01184 sprintf(footer, "attribute \"dep\" string \"positions\"\\n\" \"
01185     \"object \"regular positions regular connections\" class field\\n\" \"
01186     \"component \"positions\" value 1\\n\" \"
01187     \"component \"connections\" value 2\\n\" \"
01188     \"component \"data\" value 3\\n\"");
01189 gzwrite(outfile, footer, strlen(footer)*sizeof(char));
01190
01191 gzclose(outfile);
01192 #else
01193
01194 Vnm_print(0, "WARNING\\n");
01195 Vnm_print(0, "Vgrid_readGZ:  gzip read/write support is disabled in this build\\n");
01196 Vnm_print(0, "Vgrid_readGZ:  configure and compile without the --disable-zlib flag.\\n");
01197 Vnm_print(0, "WARNING\\n");
01198 #endif
01199 }
01200
01201 /* ////////////////////////////////////////
01202 // Routine:  Vgrid_wroteDX
01203 //
01204 // Author:   Nathan Baker
01206 VPUBLIC void Vgrid_wroteDX(Vgrid *thee, const char *iodev, const char *iofmt,
01207     const char *thost, const char *fname, char *title, double *pvec) {
01208
01209     double xmin, ymin, zmin, hx, hy, hzed;
01210     int nx, ny, nz, nxPART, nyPART, nzPART;
01211     int usepart, gotit;
01212     size_t icol, i, j, k, u;
01213     double x, y, z, xminPART, yminPART, zminPART;
01214     Vio *sock;
01215     char precFormat[VMAX_BUFSIZE];
01216
01217     if (thee == VNULL) {
01218         Vnm_print(2, "Vgrid_wroteDX:  Error -- got VNULL thee!\\n");
01219         VASSERT(0);
01220     }
01221     if (!(thee->ctordata || thee->readdata)) {
01222         Vnm_print(2, "Vgrid_wroteDX:  Error -- no data available!\\n");
01223         VASSERT(0);
01224     }
01225
01226     hx = thee->hx;
01227     hy = thee->hy;
01228     hzed = thee->hzed;
01229     nx = thee->nx;
01230     ny = thee->ny;
01231     nz = thee->nz;
01232     xmin = thee->xmin;
01233     ymin = thee->ymin;
01234     zmin = thee->zmin;
01235
01236     if (pvec == VNULL) usepart = 0;
01237     else usepart = 1;
01238
01239     /* Set up the virtual socket */
01240     Vnm_print(0, "Vgrid_wroteDX:  Opening virtual socket...\\n");
01241     sock = Vio_ctor(iodev, iofmt, thost, fname, "w");
01242     if (sock == VNULL) {
01243         Vnm_print(2, "Vgrid_wroteDX:  Problem opening virtual socket %s\\n",
01244             fname);
01245         return;
01246     }
01247     if (Vio_connect(sock, 0) < 0) {
01248         Vnm_print(2, "Vgrid_wroteDX:  Problem connecting virtual socket %s\\n",
01249             fname);
01250         return;
01251     }
01252

```

```

01253     Vio_setWhiteChars(sock, MCwhiteChars);
01254     Vio_setCommChars(sock, MCcommChars);
01255
01256     Vnm_print(0, "Vgrid_writeDX: Writing to virtual socket...\n");
01257
01258     if (usepart) {
01259         /* Get the lower corner and number of grid points for the local
01260          * partition */
01261         xminPART = VLARGE;
01262         yminPART = VLARGE;
01263         zminPART = VLARGE;
01264         nxPART = 0;
01265         nyPART = 0;
01266         nzPART = 0;
01267         /* First, search for the lower corner */
01268         for (k=0; k<nz; k++) {
01269             z = k*hzed + zmin;
01270             for (j=0; j<ny; j++) {
01271                 y = j*hy + ymin;
01272                 for (i=0; i<nx; i++) {
01273                     x = i*hx + xmin;
01274                     if (pvec[IJK(i,j,k)] > 0.0) {
01275                         if (x < xminPART) xminPART = x;
01276                         if (y < yminPART) yminPART = y;
01277                         if (z < zminPART) zminPART = z;
01278                     }
01279                 }
01280             }
01281         }
01282         /* Now search for the number of grid points in the z direction */
01283         for (k=0; k<nz; k++) {
01284             gotit = 0;
01285             for (j=0; j<ny; j++) {
01286                 for (i=0; i<nx; i++) {
01287                     if (pvec[IJK(i,j,k)] > 0.0) {
01288                         gotit = 1;
01289                         break;
01290                     }
01291                 }
01292                 if (gotit) break;
01293             }
01294             if (gotit) nzPART++;
01295         }
01296         /* Now search for the number of grid points in the y direction */
01297         for (j=0; j<ny; j++) {
01298             gotit = 0;
01299             for (k=0; k<nz; k++) {
01300                 for (i=0; i<nx; i++) {
01301                     if (pvec[IJK(i,j,k)] > 0.0) {
01302                         gotit = 1;
01303                         break;
01304                     }
01305                 }
01306                 if (gotit) break;
01307             }
01308             if (gotit) nyPART++;
01309         }
01310         /* Now search for the number of grid points in the x direction */
01311         for (i=0; i<nx; i++) {
01312             gotit = 0;
01313             for (k=0; k<nz; k++) {
01314                 for (j=0; j<ny; j++) {
01315                     if (pvec[IJK(i,j,k)] > 0.0) {
01316                         gotit = 1;
01317                         break;
01318                     }
01319                 }
01320                 if (gotit) break;
01321             }
01322             if (gotit) nxPART++;
01323         }
01324
01325         if ((nxPART != nx) || (nyPART != ny) || (nzPART != nz)) {
01326             Vnm_print(0, "Vgrid_writeDX: printing only subset of domain\n");
01327         }
01328
01329         /* Write off the title (if we're not XDR) */
01330         if (Vstring_strcasecmp(iofmt, "XDR") == 0) {
01331             Vnm_print(0, "Vgrid_writeDX: Skipping comments for XDR format.\n");
01332         } else {
01333

```

```

01334         Vnm_print(0, "Vgrid_writeDX: Writing comments for %s format.\n",
01335                     iofmt);
01336         Vio_printf(sock, "# Data from %s\n", PACKAGE_STRING);
01337         Vio_printf(sock, "# \n");
01338         Vio_printf(sock, "# %s\n", title);
01339         Vio_printf(sock, "# \n");
01340     }
01341
01342     /* Write off the DX regular positions */
01343     Vio_printf(sock, "object 1 class gridpositions counts %d %d %d\n",
01344               nxPART, nyPART, nzPART);
01345
01346     sprintf(precFormat, Vprecision, xminPART, yminPART, zminPART);
01347     Vio_printf(sock, "origin %s\n", precFormat);
01348     sprintf(precFormat, Vprecision, hx, 0.0, 0.0);
01349     Vio_printf(sock, "delta %s\n", precFormat);
01350     sprintf(precFormat, Vprecision, 0.0, hy, 0.0);
01351     Vio_printf(sock, "delta %s\n", precFormat);
01352     sprintf(precFormat, Vprecision, 0.0, 0.0, hzed);
01353     Vio_printf(sock, "delta %s\n", precFormat);
01354
01355     /* Write off the DX regular connections */
01356     Vio_printf(sock, "object 2 class gridconnections counts %d %d %d\n",
01357               nxPART, nyPART, nzPART);
01358
01359     /* Write off the DX data */
01360     Vio_printf(sock, "object 3 class array type double rank 0 items %lu \
01361 data follows\n", (nxPART*nyPART*nzPART));
01362     icol = 0;
01363     for (i=0; i<nx; i++) {
01364         for (j=0; j<ny; j++) {
01365             for (k=0; k<nz; k++) {
01366                 u = k*(nx)*(ny)+j*(nx)+i;
01367                 if (pvec[u] > 0.0) {
01368                     Vio_printf(sock, "%12.6e ", thee->data[u]);
01369                     icol++;
01370                     if (icol == 3) {
01371                         icol = 0;
01372                         Vio_printf(sock, "\n");
01373                     }
01374                 }
01375             }
01376         }
01377     }
01378
01379     if (icol != 0) Vio_printf(sock, "\n");
01380
01381     /* Create the field */
01382     Vio_printf(sock, "attribute \"dep\" string \"positions\"\n");
01383     Vio_printf(sock, "object \"regular positions regular connections\" \
01384 class field\n");
01385     Vio_printf(sock, "component \"positions\" value 1\n");
01386     Vio_printf(sock, "component \"connections\" value 2\n");
01387     Vio_printf(sock, "component \"data\" value 3\n");
01388
01389 } else {
01390     /* Write off the title (if we're not XDR) */
01391     if (Vstring_strcasecmp(iofmt, "XDR") == 0) {
01392         Vnm_print(0, "Vgrid_writeDX: Skipping comments for XDR format.\n");
01393     } else {
01394         Vnm_print(0, "Vgrid_writeDX: Writing comments for %s format.\n",
01395                     iofmt);
01396         Vio_printf(sock, "# Data from %s\n", PACKAGE_STRING);
01397         Vio_printf(sock, "# \n");
01398         Vio_printf(sock, "# %s\n", title);
01399         Vio_printf(sock, "# \n");
01400     }
01401
01402     /* Write off the DX regular positions */
01403     Vio_printf(sock, "object 1 class gridpositions counts %d %d %d\n",
01404               nx, ny, nz);
01405
01406     sprintf(precFormat, Vprecision, xmin, ymin, zmin);
01407     Vio_printf(sock, "origin %s\n", precFormat);
01408     sprintf(precFormat, Vprecision, hx, 0.0, 0.0);
01409     Vio_printf(sock, "delta %s\n", precFormat);
01410     sprintf(precFormat, Vprecision, 0.0, hy, 0.0);
01411     Vio_printf(sock, "delta %s\n", precFormat);
01412     sprintf(precFormat, Vprecision, 0.0, 0.0, hzed);
01413     Vio_printf(sock, "delta %s\n", precFormat);

```

```

01415
01416     /* Write off the DX regular connections */
01417     Vio_printf(sock, "object 2 class gridconnections counts %d %d %d\n",
01418         nx, ny, nz);
01419
01420     /* Write off the DX data */
01421     Vio_printf(sock, "object 3 class array type double rank 0 items %lu \
01422 data follows\n", (nx*ny*nz));
01423     icol = 0;
01424     for (i=0; i<nx; i++) {
01425         for (j=0; j<ny; j++) {
01426             for (k=0; k<nz; k++) {
01427                 u = k*(nx)*(ny)+j*(nx)+i;
01428                 Vio_printf(sock, "%12.6e ", thee->data[u]);
01429                 icol++;
01430                 if (icol == 3) {
01431                     icol = 0;
01432                     Vio_printf(sock, "\n");
01433                 }
01434             }
01435         }
01436     }
01437     if (icol != 0) Vio_printf(sock, "\n");
01438
01439     /* Create the field */
01440     Vio_printf(sock, "attribute \"dep\" string \"positions\"\n");
01441     Vio_printf(sock, "object \"regular positions regular connections\" \
01442 class field\n");
01443     Vio_printf(sock, "component \"positions\" value 1\n");
01444     Vio_printf(sock, "component \"connections\" value 2\n");
01445     Vio_printf(sock, "component \"data\" value 3\n");
01446 }
01447
01448     /* Close off the socket */
01449     Vio_connectFree(sock);
01450     Vio_dtor(&sock);
01451 }
01452
01453 /* ////////////////////////////////////////
01454 // Routine: Vgrid_writeDXBIN
01455 //
01456 // Author: Juan Brandi
01457 VPUBLIC void Vgrid_writeDXBIN(Vgrid *thee, const char *iodev, const char *iofmt,
01458     const char *thost, const char *fname, char *title, double *pvec){
01459
01460     double xmin, ymin, zmin, hx, hy, hzed;
01461     int nx, ny, nz, nxPART, nyPART, nzPART;
01462     int usepart, gotit;
01463     size_t icol, i, j, k, u;
01464     double x, y, z, xminPART, yminPART, zminPART;
01465     //Vio *sock;
01466     char precFormat[VMAX_BUFSIZE];
01467
01468     if (thee == VNULL) {
01469         Vnm_print(2, "Vgrid_writeDXBIN: Error -- got VNULL thee!\n");
01470         VASSERT(0);
01471     }
01472     if (!(thee->ctordata || thee->readdata)) {
01473         Vnm_print(2, "Vgrid_writeDXBIN: Error -- no data available!\n");
01474         VASSERT(0);
01475     }
01476
01477
01478
01479     hx = thee->hx;
01480     hy = thee->hy;
01481     hzed = thee->hzed;
01482     nx = thee->nx;
01483     ny = thee->ny;
01484     nz = thee->nz;
01485     xmin = thee->xmin;
01486     ymin = thee->ymin;
01487     zmin = thee->zmin;
01488
01489     if (pvec == VNULL) usepart = 0;
01490     else usepart = 1;
01491
01492     /*will not use vio methods to try to avoid using malloc.*/
01493     FILE *fd = fopen(fname, "wb");
01494
01495     //check to se if the file was created/open successfully.
01496     if (fd == NULL){

```

```

01497     printf("Vgrid_writeDXBIN: Problem opening file %s for writing.\n", fname);
01498     return;
01499 }
01500
01501 printf("Vgrid_writeDXBIN: Writing to file...\n");
01502
01503 if (usepart) {
01504     /* Get the lower corner and number of grid points for the local
01505      * partition */
01506     xminPART = VLARGE;
01507     yminPART = VLARGE;
01508     zminPART = VLARGE;
01509     nxPART = 0;
01510     nyPART = 0;
01511     nzPART = 0;
01512     /* First, search for the lower corner */
01513     for (k=0; k<nz; k++) {
01514         z = k*hzed + zmin;
01515         for (j=0; j<ny; j++) {
01516             y = j*hy + ymin;
01517             for (i=0; i<nx; i++) {
01518                 x = i*hx + xmin;
01519                 if (pvec[IJK(i,j,k)] > 0.0) {
01520                     if (x < xminPART) xminPART = x;
01521                     if (y < yminPART) yminPART = y;
01522                     if (z < zminPART) zminPART = z;
01523                 }
01524             }
01525         }
01526     }
01527     /* Now search for the number of grid points in the z direction */
01528     for (k=0; k<nz; k++) {
01529         gotit = 0;
01530         for (j=0; j<ny; j++) {
01531             for (i=0; i<nx; i++) {
01532                 if (pvec[IJK(i,j,k)] > 0.0) {
01533                     gotit = 1;
01534                     break;
01535                 }
01536             }
01537             if (gotit) break;
01538         }
01539         if (gotit) nzPART++;
01540     }
01541     /* Now search for the number of grid points in the y direction */
01542     for (j=0; j<ny; j++) {
01543         gotit = 0;
01544         for (k=0; k<nz; k++) {
01545             for (i=0; i<nx; i++) {
01546                 if (pvec[IJK(i,j,k)] > 0.0) {
01547                     gotit = 1;
01548                     break;
01549                 }
01550             }
01551             if (gotit) break;
01552         }
01553         if (gotit) nyPART++;
01554     }
01555     /* Now search for the number of grid points in the x direction */
01556     for (i=0; i<nx; i++) {
01557         gotit = 0;
01558         for (k=0; k<nz; k++) {
01559             for (j=0; j<ny; j++) {
01560                 if (pvec[IJK(i,j,k)] > 0.0) {
01561                     gotit = 1;
01562                     break;
01563                 }
01564             }
01565             if (gotit) break;
01566         }
01567         if (gotit) nxPART++;
01568     }
01569
01570     if ((nxPART != nx) || (nyPART != ny) || (nzPART != nz)) {
01571         Vnm_print(0, "Vgrid_writeDXBIN: printing only subset of domain\n");
01572     }
01573
01574     /* Write title (we're in XDR and "wb") */
01575     //Vnm_print(0, "Vgrid_writeDXBIN: Writing comments for dxbin format.\n");
01576     printf("Vgrid_writeDXBIN: Writing comments for dxbin format\n");
01577     fprintf(fd, "# Data from %s\n", PACKAGE_STRING);

```

```

01578     fprintf(fd, "# \n");
01579     fprintf(fd, "# %s\n",title);
01580     fprintf(fd, "# \n");
01581
01582     /* Write off the DX regular positions */
01583     fprintf(fd, "object 1 class gridpositions counts %d %d %d\n",nxPART, nyPART, nzPART);
01584
01585     sprintf(precFormat, Vprecision, xminPART, yminPART, zminPART);
01586     fprintf(fd, "origin %s\n",precFormat);
01587
01588     sprintf(precFormat, Vprecision, hx, 0.0, 0.0);
01589     fprintf(fd, "delta %s\n",precFormat);
01590
01591     sprintf(precFormat, Vprecision, 0.0, hy, 0.0);
01592     fprintf(fd, "delta %s\n", precFormat);
01593
01594     sprintf(precFormat, Vprecision, 0.0, 0.0, hzed);
01595     fprintf(fd, "delta %s\n", precFormat);
01596
01597     /* Write off the DX regular connections */
01598     fprintf(fd, "object 2 class gridconnections counts %d %d %d\n", nxPART, nyPART, nzPART);
01599
01600     /* Write off the DX data */
01601     fprintf(fd, "object 3 class array type double rank 0 items %d binary data
follows\n", (nxPART*nyPART*nzPART));
01602
01603     icol = 0;
01604     for (i=0; i<nx; i++) {
01605         for (j=0; j<ny; j++) {
01606             for (k=0; k<nz; k++) {
01607                 u = k*(nx)*(ny)+j*(nx)+i;
01608                 if (pvec[u] > 0.0) {
01609                     fwrite(&(thee->data)[u],sizeof(double),1,fd);
01610                     icol++;
01611                     /*don't need the column formating to write binary doubles.*/
01612                     if (icol == 3) {
01613                         icol = 0;
01614                     }
01615                 }
01616             }
01617         }
01618     }
01619
01620     fprintf(fd, "\n");
01621
01622     /* Create the field */
01623     fprintf(fd, "attribute \"dep\" string \"positions\"\n");
01624     fprintf(fd, "object \"regular positions regular connections\" class field\n");
01625     fprintf(fd, "component \"positions\" value 1\n");
01626     fprintf(fd, "component \"connections\" value 2\n");
01627     fprintf(fd, "component \"data\" value 3\n");
01628
01629     fclose(fd);
01630
01631 } else {
01632     /*write dx format title*/
01633     printf("Vgrid_writeDXBIN: Writing comments for %s format.\n",iofmt);
01634     fprintf(fd,"# Data from %s\n", PACKAGE_STRING);
01635     fprintf(fd,"# \n");
01636     fprintf(fd, "# %s\n", title);
01637     fprintf(fd, "# \n");
01638
01639     /* Write off the DX regular positions */
01640     fprintf(fd, "object 1 class gridpositions counts %d %d %d\n", nx, ny, nz);
01641
01642     sprintf(precFormat, Vprecision, xmin, ymin, zmin);
01643     fprintf(fd, "origin %s\n", precFormat);
01644
01645     sprintf(precFormat, Vprecision, hx, 0.0, 0.0);
01646     fprintf(fd, "delta %s\n", precFormat);
01647
01648     sprintf(precFormat, Vprecision, 0.0, hy, 0.0);
01649     fprintf(fd, "delta %s\n", precFormat);
01650
01651     sprintf(precFormat, Vprecision, 0.0, 0.0, hzed);
01652     fprintf(fd, "delta %s\n", precFormat);
01653
01654     /* Write off the DX regular connections */
01655     fprintf(fd, "object 2 class gridconnections counts %d %d %d\n", nx, ny, nz);
01656
01657     /* Write off the DX data */

```



```

01658     fprintf(fd, "object 3 class array type double rank 0 items %d binary data follows\n", (nx*ny*nz));
01659
01660     icol = 0;
01661     for (i=0; i<nx; i++) {
01662         for (j=0; j<ny; j++) {
01663             for (k=0; k<nz; k++) {
01664                 u = k*(nx)*(ny)+j*(nx)+i;
01665                 fwrite(&(thee->data)[u], sizeof(double), 1, fd);
01666                 icol++;
01667                 if (icol == 3) {
01668                     icol = 0;
01669                 }
01670             }
01671         }
01672     }
01673
01674     fprintf(fd, "\n");
01675
01676     /* Create the field */
01677     fprintf(fd, "attribute \"dep\" string \"positions\"\n");
01678     fprintf(fd, "object \"regular positions regular connections\" class field\n");
01679     fprintf(fd, "component \"positions\" value 1\n");
01680     fprintf(fd, "component \"connections\" value 2\n");
01681     fprintf(fd, "component \"data\" value 3\n");
01682
01683     fclose(fd);
01684 }
01685 }
01686
01687
01688 /* ////////////////////////////////////////
01689 // Routine:  Vgrid_writeUHBD
01690 // Author:   Nathan Baker
01692 VPUBLIC void Vgrid_writeUHBD(Vgrid *thee, const char *iodev, const char *iofmt,
01693     const char *thost, const char *fname, char *title, double *pvec) {
01694
01695     size_t u, icol, i, j, k;
01696     size_t gotit, nx, ny, nz;
01697     double xmin, ymin, zmin, hzed, hy, hx;
01698     Vio *sock;
01699
01700     if (thee == VNULL) {
01701         Vnm_print(2, "Vgrid_writeUHBD: Error -- got VNULL thee!\n");
01702         VASSERT(0);
01703     }
01704     if (!(thee->ctordata || thee->readdata)) {
01705         Vnm_print(2, "Vgrid_writeUHBD: Error -- no data available!\n");
01706         VASSERT(0);
01707     }
01708
01709     if ((thee->hx!=thee->hy) || (thee->hy!=thee->hzed)
01710         || (thee->hx!=thee->hzed)) {
01711         Vnm_print(2, "Vgrid_writeUHBD: can't write UHBD mesh with non-uniform \
01712 spacing\n");
01713         return;
01714     }
01715
01716     /* Set up the virtual socket */
01717     sock = Vio_ctor(iodev, iofmt, thost, fname, "w");
01718     if (sock == VNULL) {
01719         Vnm_print(2, "Vgrid_writeUHBD: Problem opening virtual socket %s\n",
01720             fname);
01721         return;
01722     }
01723     if (Vio_connect(sock, 0) < 0) {
01724         Vnm_print(2, "Vgrid_writeUHBD: Problem connecting virtual socket %s\n",
01725             fname);
01726         return;
01727     }
01728
01729     /* Get the lower corner and number of grid points for the local
01730      * partition */
01731     hx = thee->hx;
01732     hy = thee->hy;
01733     hzed = thee->hzed;
01734     nx = thee->nx;
01735     ny = thee->ny;
01736     nz = thee->nz;
01737     xmin = thee->xmin;
01738     ymin = thee->ymin;
01739     zmin = thee->zmin;

```

```

01740
01741 /* Let interested folks know that partition information is ignored */
01742 if (pvec != VNULL) {
01743     gotit = 0;
01744     for (i=0; i<(nx*ny*nz); i++) {
01745         if (pvec[i] == 0) {
01746             gotit = 1;
01747             break;
01748         }
01749     }
01750     if (gotit) {
01751         Vnm_print(2, "Vgrid_writeUHBD:  IGNORING PARTITION INFORMATION!\n");
01752         Vnm_print(2, "Vgrid_writeUHBD:  This means I/O from parallel runs \
01753 will have significant overlap.\n");
01754     }
01755 }
01756
01757 /* Write out the header */
01758 Vio_printf(sock, "%72s\n", title);
01759 Vio_printf(sock, "%12.5e%12.5e%7d%7d%7d%7d\n", 1.0, 0.0, -1, 0,
01760 nz, 1, nz);
01761 Vio_printf(sock, "%7d%7d%7d%12.5e%12.5e%12.5e%12.5e\n", nx, ny, nz,
01762 hx, (xmin-hx), (ymin-hx), (zmin-hx));
01763 Vio_printf(sock, "%12.5e%12.5e%12.5e%12.5e\n", 0.0, 0.0, 0.0, 0.0);
01764 Vio_printf(sock, "%12.5e%12.5e%7d%7d", 0.0, 0.0, 0, 0);
01765
01766 /* Write out the entries */
01767 icol = 0;
01768 for (k=0; k<nz; k++) {
01769     Vio_printf(sock, "\n%7d%7d%7d\n", k+1, thee->nx, thee->ny);
01770     icol = 0;
01771     for (j=0; j<ny; j++) {
01772         for (i=0; i<nx; i++) {
01773             u = k*(nx)*(ny)+j*(nx)+i;
01774             icol++;
01775             Vio_printf(sock, " %12.5e", thee->data[u]);
01776             if (icol == 6) {
01777                 icol = 0;
01778                 Vio_printf(sock, "\n");
01779             }
01780         }
01781     }
01782 }
01783 if (icol != 0) Vio_printf(sock, "\n");
01784
01785 /* Close off the socket */
01786 Vio_connectFree(sock);
01787 Vio_dtor(&sock);
01788 }
01789
01790 VPUBLIC double Vgrid_integrate(Vgrid *thee) {
01791
01792     size_t i, j, k;
01793     int nx, ny, nz;
01794     double sum, w;
01795
01796     if (thee == VNULL) {
01797         Vnm_print(2, "Vgrid_integrate:  Got VNULL thee!\n");
01798         VASSERT(0);
01799     }
01800
01801     nx = thee->nx;
01802     ny = thee->ny;
01803     nz = thee->nz;
01804
01805     sum = 0.0;
01806
01807     for (k=0; k<nz; k++) {
01808         w = 1.0;
01809         if ((k==0) || (k==(nz-1))) w = w * 0.5;
01810         for (j=0; j<ny; j++) {
01811             w = 1.0;
01812             if ((j==0) || (j==(ny-1))) w = w * 0.5;
01813             for (i=0; i<nx; i++) {
01814                 w = 1.0;
01815                 if ((i==0) || (i==(nx-1))) w = w * 0.5;
01816                 sum = sum + w*(thee->data[IJK(i,j,k)]);
01817             }
01818         }
01819     }
01820

```

```

01821     sum = sum*(thee->hx)*(thee->hy)*(thee->hz);
01822
01823     return sum;
01824 }
01825 }
01826
01827
01828 VPUBLIC double Vgrid_normL1(Vgrid *thee) {
01829
01830     size_t i, j, k;
01831     int nx, ny, nz;
01832     double sum;
01833
01834     if (thee == VNULL) {
01835         Vnm_print(2, "Vgrid_normL1: Got VNULL thee!\n");
01836         VASSERT(0);
01837     }
01838
01839     nx = thee->nx;
01840     ny = thee->ny;
01841     nz = thee->nz;
01842
01843     sum = 0.0;
01844     for (k=0; k<nz; k++) {
01845         for (j=0; j<ny; j++) {
01846             for (i=0; i<nx; i++) {
01847                 sum = sum + VABS(thee->data[IJK(i,j,k)]);
01848             }
01849         }
01850     }
01851
01852     sum = sum*(thee->hx)*(thee->hy)*(thee->hz);
01853
01854     return sum;
01855 }
01856 }
01857
01858 VPUBLIC double Vgrid_normL2(Vgrid *thee) {
01859
01860     size_t i, j, k;
01861     int nx, ny, nz;
01862     double sum;
01863
01864     if (thee == VNULL) {
01865         Vnm_print(2, "Vgrid_normL2: Got VNULL thee!\n");
01866         VASSERT(0);
01867     }
01868
01869     nx = thee->nx;
01870     ny = thee->ny;
01871     nz = thee->nz;
01872
01873     sum = 0.0;
01874     for (k=0; k<nz; k++) {
01875         for (j=0; j<ny; j++) {
01876             for (i=0; i<nx; i++) {
01877                 sum = sum + VSQR(thee->data[IJK(i,j,k)]);
01878             }
01879         }
01880     }
01881
01882     sum = sum*(thee->hx)*(thee->hy)*(thee->hz);
01883
01884     return VSQRT(sum);
01885 }
01886 }
01887
01888 VPUBLIC double Vgrid_seminormH1(Vgrid *thee) {
01889
01890     size_t i, j, k;
01891     int nx, ny, nz, d;
01892     double pt[3], grad[3], sum, hx, hy, hzed, xmin, ymin, zmin;
01893
01894     if (thee == VNULL) {
01895         Vnm_print(2, "Vgrid_seminormH1: Got VNULL thee!\n");
01896         VASSERT(0);
01897     }
01898
01899     nx = thee->nx;
01900     ny = thee->ny;
01901     nz = thee->nz;

```

```

01902     hx = thee->hx;
01903     hy = thee->hy;
01904     hzed = thee->hzed;
01905     xmin = thee->xmin;
01906     ymin = thee->ymin;
01907     zmin = thee->zmin;
01908
01909     sum = 0.0;
01910     for (k=0; k<nz; k++) {
01911         pt[2] = k*hzed + zmin;
01912         for (j=0; j<ny; j++) {
01913             pt[1] = j*hy + ymin;
01914             for (i=0; i<nx; i++) {
01915                 pt[0] = i*hx + xmin;
01916                 VASSERT(Vgrid_gradient(thee, pt, grad));
01917                 for (d=0; d<3; d++) sum = sum + VSQR(grad[d]);
01918             }
01919         }
01920     }
01921
01922     sum = sum*(hx)*(hy)*(hzed);
01923
01924     if (VABS(sum) < VSMALL) sum = 0.0;
01925     else sum = VSQRT(sum);
01926
01927     return sum;
01928 }
01929
01930
01931 VPUBLIC double Vgrid_normH1(Vgrid *thee) {
01932     double sum = 0.0;
01933
01934     if (thee == VNULL) {
01935         Vnm_print(2, "Vgrid_normH1: Got VNULL thee!\n");
01936         VASSERT(0);
01937     }
01938
01939     sum = VSQR(Vgrid_seminormH1(thee)) + VSQR(Vgrid_normL2(thee));
01940
01941     return VSQRT(sum);
01942 }
01943
01944
01945
01946 VPUBLIC double Vgrid_normLinf(Vgrid *thee) {
01947     size_t i, j, k;
01948     int nx, ny, nz, gotval;
01949     double sum, val;
01950
01951     if (thee == VNULL) {
01952         Vnm_print(2, "Vgrid_normLinf: Got VNULL thee!\n");
01953         VASSERT(0);
01954     }
01955
01956     nx = thee->nx;
01957     ny = thee->ny;
01958     nz = thee->nz;
01959
01960     sum = 0.0;
01961     gotval = 0;
01962     for (k=0; k<nz; k++) {
01963         for (j=0; j<ny; j++) {
01964             for (i=0; i<nx; i++) {
01965                 val = VABS(thee->data[IJK(i,j,k)]);
01966                 if (!gotval) {
01967                     gotval = 1;
01968                     sum = val;
01969                 }
01970                 if (val > sum) sum = val;
01971             }
01972         }
01973     }
01974
01975     return sum;
01976 }
01977
01978 }

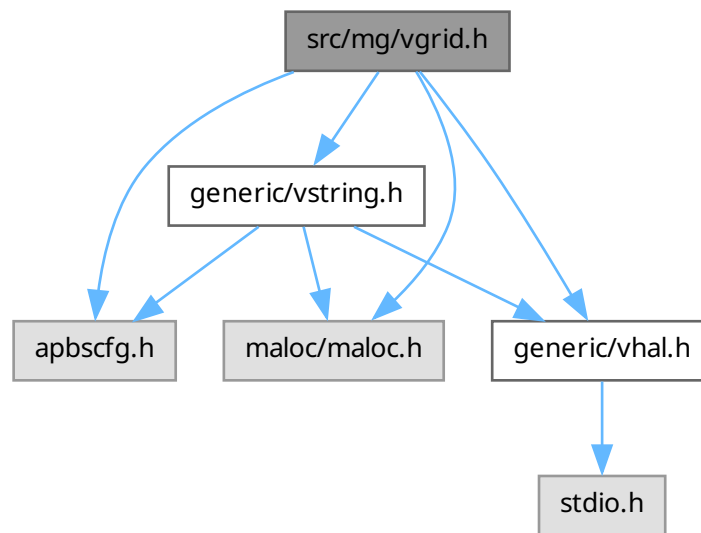
```

9.96 src/mg/vgrid.h File Reference

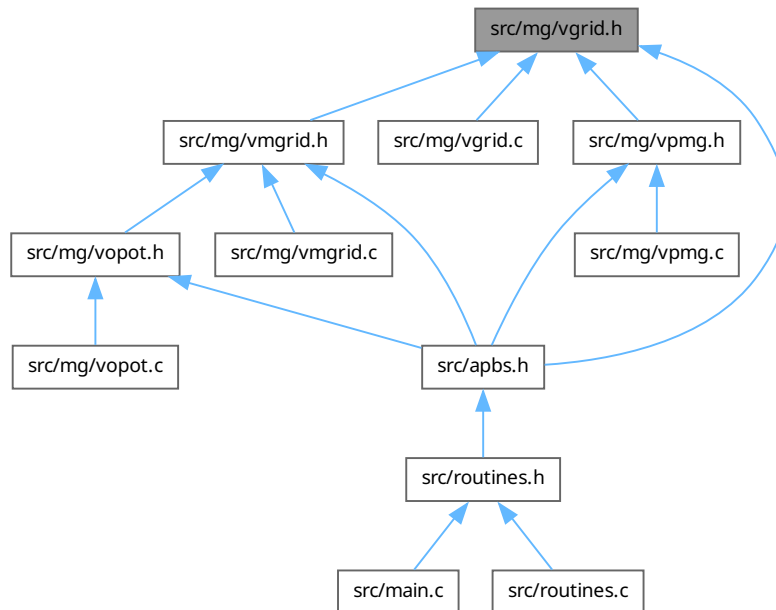
Potential oracle for Cartesian mesh data.

```
#include "apbscfg.h"  
#include "malloc/malloc.h"  
#include "generic/vhal.h"  
#include "generic/vstring.h"
```

Include dependency graph for vgrid.h:



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [sVgrid](#)
Electrostatic potential oracle for Cartesian mesh data.

Macros

- #define [VGRID_DIGITS](#) 6
Number of decimal places for comparisons and formatting.

Typedefs

- typedef struct [sVgrid](#) [Vgrid](#)
Declaration of the Vgrid class as the [sVgrid](#) structure.

Functions

- VEXTERNC unsigned long int [Vgrid_memChk](#) ([Vgrid](#) *thee)
Return the memory used by this structure (and its contents) in bytes.
- VEXTERNC [Vgrid](#) * [Vgrid_ctor](#) (int nx, int ny, int nz, double hx, double hy, double hzed, double xmin, double ymin, double zmin, double *data)
Construct Vgrid object with values obtained from Vpmg_readDX (for example)
- VEXTERNC int [Vgrid_ctor2](#) ([Vgrid](#) *thee, int nx, int ny, int nz, double hx, double hy, double hzed, double xmin, double ymin, double zmin, double *data)
Initialize Vgrid object with values obtained from Vpmg_readDX (for example)

- VEXTERNC int [Vgrid_value](#) ([Vgrid](#) *thee, double x[3], double *value)
Get potential value (from mesh or approximation) at a point.
- VEXTERNC void [Vgrid_dtor](#) ([Vgrid](#) **thee)
Object destructor.
- VEXTERNC void [Vgrid_dtor2](#) ([Vgrid](#) *thee)
FORTTRAN stub object destructor.
- VEXTERNC int [Vgrid_curvature](#) ([Vgrid](#) *thee, double pt[3], int cflag, double *curv)
Get second derivative values at a point.
- VEXTERNC int [Vgrid_gradient](#) ([Vgrid](#) *thee, double pt[3], double grad[3])
Get first derivative values at a point.
- VEXTERNC int [Vgrid_readGZ](#) ([Vgrid](#) *thee, const char *fname)
Read in OpenDX data in GZIP format.
- VEXTERNC void [Vgrid_writeGZ](#) ([Vgrid](#) *thee, const char *iodev, const char *iofmt, const char *thost, const char *fname, char *title, double *pvec)
Write out OpenDX data in GZIP format.
- VEXTERNC void [Vgrid_writeUHBD](#) ([Vgrid](#) *thee, const char *iodev, const char *iofmt, const char *thost, const char *fname, char *title, double *pvec)
Write out the data in UHBD grid format.
- VEXTERNC void [Vgrid_writeDX](#) ([Vgrid](#) *thee, const char *iodev, const char *iofmt, const char *thost, const char *fname, char *title, double *pvec)
Write out the data in OpenDX grid format.
- VEXTERNC int [Vgrid_readDX](#) ([Vgrid](#) *thee, const char *iodev, const char *iofmt, const char *thost, const char *fname)
Read in data in OpenDX grid format.
- VEXTERNC void [Vgrid_writeDXBIN](#) ([Vgrid](#) *thee, const char *iodev, const char *iofmt, const char *thost, const char *fname, char *title, double *pvec)
Write out the binary data in OpenDX grid format.
- VEXTERNC int [Vgrid_readDXBIN](#) ([Vgrid](#) *thee, const char *iodev, const char *iofmt, const char *thost, const char *fname)
Read in binary data in OpenDX grid format.
- VEXTERNC double [Vgrid_integrate](#) ([Vgrid](#) *thee)
Get the integral of the data.
- VEXTERNC double [Vgrid_normL1](#) ([Vgrid](#) *thee)
Get the L_1 norm of the data. This returns the integral:
- VEXTERNC double [Vgrid_normL2](#) ([Vgrid](#) *thee)
Get the L_2 norm of the data. This returns the integral:
- VEXTERNC double [Vgrid_normLinf](#) ([Vgrid](#) *thee)
Get the L_∞ norm of the data. This returns the integral:
- VEXTERNC double [Vgrid_seminormH1](#) ([Vgrid](#) *thee)
Get the H_1 semi-norm of the data. This returns the integral:
- VEXTERNC double [Vgrid_normH1](#) ([Vgrid](#) *thee)
Get the H_1 norm (or energy norm) of the data. This returns the integral:

9.96.1 Detailed Description

Potential oracle for Cartesian mesh data.

Author

Nathan Baker and Steve Bond

Version

\$Id\$

Attention

```
*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
*   Nathan A. Baker (nathan.baker@pnnl.gov)
*   Pacific Northwest National Laboratory
*
*   Additional contributing authors listed in the code documentation.
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* THE POSSIBILITY OF SUCH DAMAGE.
*
*
```

Definition in file [vgrid.h](#).

9.96.2 Function Documentation

9.96.2.1 Vgrid_writeGZ()

```
VEXTERNC void Vgrid_writeGZ (
```



```

Vgrid * thee,
const char * iodev,
const char * iofmt,
const char * thost,
const char * fname,
char * title,
double * pvec )

```

Write out OpenDX data in GZIP format.

Author

Dave Gohara

Parameters

<i>thee</i>	Object to hold new grid data
<i>iodev</i>	I/O device
<i>iofmt</i>	I/O format
<i>thost</i>	Remote host name
<i>fname</i>	File name
<i>title</i>	Data title
<i>pvec</i>	Masking vector (0 = not written)

Definition at line 1011 of file [vgrid.c](#).

9.97 vgrid.h

[Go to the documentation of this file.](#)

```

00001
00062 #ifndef _VGRID_H_
00063 #define _VGRID_H_
00064
00065 #include "apbscfg.h"
00066
00067 #include "malloc/malloc.h"
00068
00069 #include "generic/vhal.h"
00070 #include "generic/vstring.h"
00071
00074 #define VGRID_DIGITS 6
00075
00081 struct sVgrid {
00082
00083     int nx;
00084     int ny;
00085     int nz;
00086     double hx;
00087     double hy;
00088     double hzed;
00089     double xmin;
00090     double ymin;
00091     double zmin;
00092     double xmax;
00093     double ymax;
00094     double zmax;
00095     double *data;
00096     int readdata;
00097     int ctordata;
00099     Vmem *mem;
00100 };
00101
00106 typedef struct sVgrid Vgrid;
00107
00108 #if !defined(VINLINE_VGRID)
00109

```

```

00117     VEXTERNC unsigned long int Vgrid_memChk(Vgrid *thee);
00118
00119 #else /* if defined(VINLINE_VGRID) */
00120
00128 #define Vgrid_memChk(thee) (Vmem_bytes((thee)->vmem))
00129
00130 #endif /* if !defined(VINLINE_VPMG) */
00131
00149 VEXTERNC Vgrid* Vgrid_ctor(int nx, int ny, int nz,
00150                             double hx, double hy, double hzed,
00151                             double xmin, double ymin, double zmin,
00152                             double *data);
00153
00172 VEXTERNC int Vgrid_ctor2(Vgrid *thee, int nx, int ny, int nz,
00173                          double hx, double hy, double hzed,
00174                          double xmin, double ymin, double zmin,
00175                          double *data);
00176
00185 VEXTERNC int Vgrid_value(Vgrid *thee, double x[3], double *value);
00186
00192 VEXTERNC void Vgrid_dtor(Vgrid **thee);
00193
00199 VEXTERNC void Vgrid_dtor2(Vgrid *thee);
00200
00214 VEXTERNC int Vgrid_curvature(Vgrid *thee, double pt[3], int cflag,
00215                             double *curv);
00216
00225 VEXTERNC int Vgrid_gradient(Vgrid *thee, double pt[3], double grad[3] );
00226
00231 VEXTERNC int Vgrid_readGZ(
00232     Vgrid *thee,
00233     const char *fname
00234 );
00235
00239 VEXTERNC void Vgrid_writeGZ(
00240     Vgrid *thee,
00241     const char *iodev,
00242     const char *iofmt,
00243     const char *thost,
00244     const char *fname,
00245     char *title,
00246     double *pvec
00247 );
00248
00266 VEXTERNC void Vgrid_writeUHBD(Vgrid *thee, const char *iodev,
00267                                const char *iofmt, const char *thost, const char *fname, char *title,
00268                                double *pvec);
00269
00284 VEXTERNC void Vgrid_writeDX(Vgrid *thee, const char *iodev,
00285                                const char *iofmt, const char *thost, const char *fname, char *title,
00286                                double *pvec);
00287
00299 VEXTERNC int Vgrid_readDX(Vgrid *thee, const char *iodev, const char *iofmt,
00300                             const char *thost, const char *fname);
00301
00316 VEXTERNC void Vgrid_writeDXBIN(Vgrid *thee, const char *iodev,
00317                                const char *iofmt, const char *thost, const char *fname, char *title,
00318                                double *pvec);
00319
00320
00332 VEXTERNC int Vgrid_readDXBIN(Vgrid *thee, const char *iodev, const char *iofmt,
00333                                const char *thost, const char *fname);
00334
00341 VEXTERNC double Vgrid_integrate(Vgrid *thee);
00342
00351 VEXTERNC double Vgrid_normL1(Vgrid *thee);
00352
00361 VEXTERNC double Vgrid_normL2(Vgrid *thee);
00362
00371 VEXTERNC double Vgrid_normLinf(Vgrid *thee);
00372
00382 VEXTERNC double Vgrid_seminormH1(Vgrid *thee);
00383
00394 VEXTERNC double Vgrid_normH1(Vgrid *thee);
00395
00396 #endif

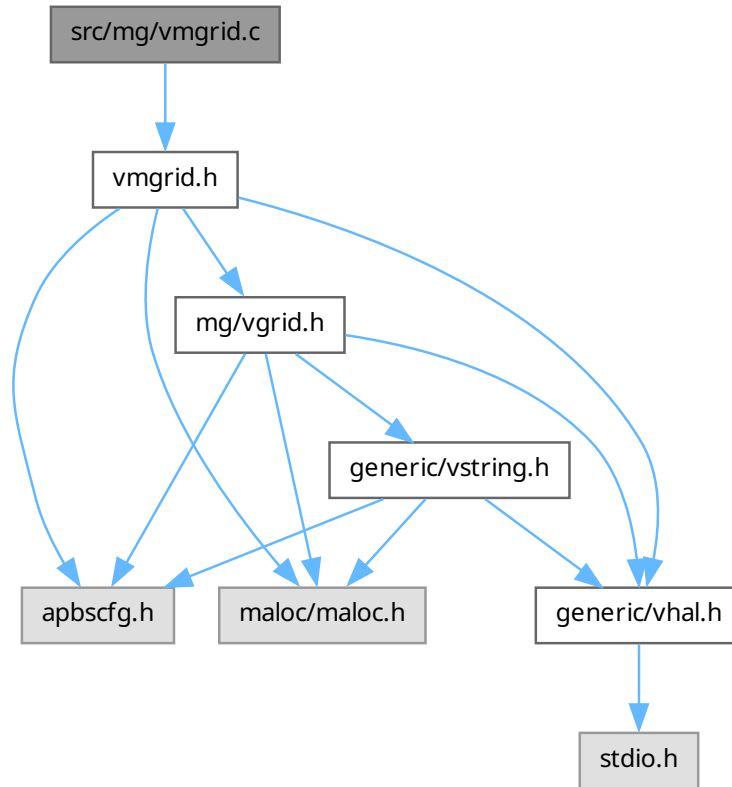
```

9.98 src/mg/vmgrid.c File Reference

Class Vmgrid methods.

```
#include "vmgrid.h"
```

Include dependency graph for vmgrid.c:



Functions

- `VPUBLIC Vmgrid * Vmgrid_ctor ()`
Construct Vmgrid object.
- `VPUBLIC int Vmgrid_ctor2 (Vmgrid *thee)`
Initialize Vmgrid object.
- `VPUBLIC void Vmgrid_dtor (Vmgrid **thee)`
Object destructor.
- `VPUBLIC void Vmgrid_dtor2 (Vmgrid *thee)`
FORTTRAN stub object destructor.
- `VPUBLIC int Vmgrid_value (Vmgrid *thee, double pt[3], double *value)`
Get potential value (from mesh or approximation) at a point.
- `VPUBLIC int Vmgrid_curvature (Vmgrid *thee, double pt[3], int cflag, double *value)`
Get second derivative values at a point.

- VPUBLIC int [Vmgrid_gradient](#) ([Vmgrid](#) *thee, double pt[3], double grad[3])
Get first derivative values at a point.
- VPUBLIC int [Vmgrid_addGrid](#) ([Vmgrid](#) *thee, [Vgrid](#) *grid)
Add a grid to the hierarchy.

9.98.1 Detailed Description

Class Vmgrid methods.

Author

Nathan Baker

Version

Id

[vmgrid.c](#) 1615 2010-10-20 19:16:35Z sobolevnm

Attention

```
*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
* Nathan A. Baker (nathan.baker@pnl.gov)
* Pacific Northwest National Laboratory
*
* Additional contributing authors listed in the code documentation.
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*
*
```

Definition in file [vmgrid.c](#).

9.99 vmgrid.c

[Go to the documentation of this file.](#)

```

00001
00049 #include "vmgrid.h"
00050
00051 VEMBED(rcsid="$Id: vmgrid.c 1615 2010-10-20 19:16:35Z sobolevnmr $")
00052
00053 /* ////////////////////////////////////////////////////////////////////
00054 // Routine:  Vmgrid_ctor
00055 // Author:   Nathan Baker
00057 VPUBLIC Vmgrid* Vmgrid_ctor() {
00058
00059     Vmgrid *thee = VNULL;
00060
00061     thee = Vmem_malloc(VNULL, 1, sizeof(Vmgrid));
00062     VASSERT(thee != VNULL);
00063     VASSERT(Vmgrid_ctor2(thee));
00064
00065     return thee;
00066 }
00067
00068 /* ////////////////////////////////////////////////////////////////////
00069 // Routine:  Vmgrid_ctor2
00070 // Author:   Nathan Baker
00072 VPUBLIC int Vmgrid_ctor2(Vmgrid *thee) {
00073
00074     int i;
00075
00076     if (thee == VNULL) return 0;
00077
00078     thee->ngrids = 0;
00079     for (i=0; i<VMGRIDMAX; i++) thee->grids[i] = VNULL;
00080
00081     return 1;
00082 }
00083
00084 /* ////////////////////////////////////////////////////////////////////
00085 // Routine:  Vmgrid_dtor
00086 // Author:   Nathan Baker
00088 VPUBLIC void Vmgrid_dtor(Vmgrid **thee) {
00089
00090     if ((*thee) != VNULL) {
00091         Vmgrid_dtor2(*thee);
00092         Vmem_free(VNULL, 1, sizeof(Vmgrid), (void **)thee);
00093         (*thee) = VNULL;
00094     }
00095 }
00096
00097 /* ////////////////////////////////////////////////////////////////////
00098 // Routine:  Vmgrid_dtor2
00099 // Author:   Nathan Baker
00101 VPUBLIC void Vmgrid_dtor2(Vmgrid *thee) { ; }
00102
00103 /* ////////////////////////////////////////////////////////////////////
00104 // Routine:  Vmgrid_value
00105 // Author:   Nathan Baker
00107 VPUBLIC int Vmgrid_value(Vmgrid *thee, double pt[3], double *value) {
00108
00109     int i, rc;
00110     double tvalue;
00111
00112     VASSERT(thee != VNULL);
00113
00114     for (i=0; i<thee->ngrids; i++) {
00115         rc = Vgrid_value(thee->grids[i], pt, &tvalue);
00116         if (rc) {
00117             *value = tvalue;
00118             return 1;
00119         }
00120     }
00121
00122     Vnm_print(2, "Vmgrid_value: Point (%g, %g, %g) not found in \
00123 hierarchy!\n", pt[0], pt[1], pt[2]);
00124
00125     return 0;
00126 }
00127
00128 /* ////////////////////////////////////////////////////////////////////
00129 // Routine:  Vmgrid_curvature

```

```

00130 //
00131 //   Notes:  cflag=0 ==> Reduced Maximal Curvature
00132 //           cflag=1 ==> Mean Curvature (Laplace)
00133 //           cflag=2 ==> Gauss Curvature
00134 //           cflag=3 ==> True Maximal Curvature
00135 //
00136 // Authors:  Nathan Baker
00138 VPUBLIC int Vmgrid_curvature(Vmgrid *thee, double pt[3], int cflag,
00139     double *value) {
00140
00141     int i, rc;
00142     double tvalue;
00143
00144     VASSERT(thee != VNULL);
00145
00146     for (i=0; i<thee->ngrids; i++) {
00147         rc = Vgrid_curvature(thee->grids[i], pt, cflag, &tvalue);
00148         if (rc) {
00149             *value = tvalue;
00150             return 1;
00151         }
00152     }
00153
00154     Vnm_print(2, "Vmgrid_curvature:  Point (%g, %g, %g) not found in \
00155 hierarchy!\n", pt[0], pt[1], pt[2]);
00156
00157     return 0;
00158
00159 }
00160
00161 /* ////////////////////////////////////////
00162 // Routine:  Vmgrid_gradient
00163 //
00164 // Authors:  Nathan Baker
00167 VPUBLIC int Vmgrid_gradient(Vmgrid *thee, double pt[3], double grad[3]) {
00168
00169     int i, j, rc;
00170     double tgrad[3];
00171
00172     VASSERT(thee != VNULL);
00173
00174     for (i=0; i<thee->ngrids; i++) {
00175         rc = Vgrid_gradient(thee->grids[i], pt, tgrad);
00176         if (rc) {
00177             for (j=0; j<3; j++) grad[j] = tgrad[j];
00178             return 1;
00179         }
00180     }
00181
00182     Vnm_print(2, "Vmgrid_gradient:  Point (%g, %g, %g) not found in \
00183 hierarchy!\n", pt[0], pt[1], pt[2]);
00184
00185     return 0;
00186
00187 }
00188
00189 /* ////////////////////////////////////////
00190 // Routine:  Vmgrid_addGrid
00191 //
00192 // Authors:  Nathan Baker
00195 VPUBLIC int Vmgrid_addGrid(Vmgrid *thee, Vgrid *grid) {
00196
00197     int i, j, rc;
00198     double tgrad[3];
00199
00200     VASSERT(thee != VNULL);
00201
00202     if (grid == VNULL) {
00203         Vnm_print(2, "Vmgrid_addGrid:  Not adding VNULL grid!\n");
00204         return 0;
00205     }
00206
00207     if (thee->ngrids >= VMGRIDMAX) {
00208         Vnm_print(2, "Vmgrid_addGrid:  Too many grids in hierarchy (max = \
00209 %d)!\n", VMGRIDMAX);
00210         Vnm_print(2, "Vmgrid_addGrid:  Not adding grid!\n");
00211         return 0;
00212     }
00213

```

```

00214     thee->grids[thee->ngrids] = grid;
00215     (thee->ngrids)++;
00216
00217     return 1;
00218
00219 }

```

9.100 src/mg/vmgrid.h File Reference

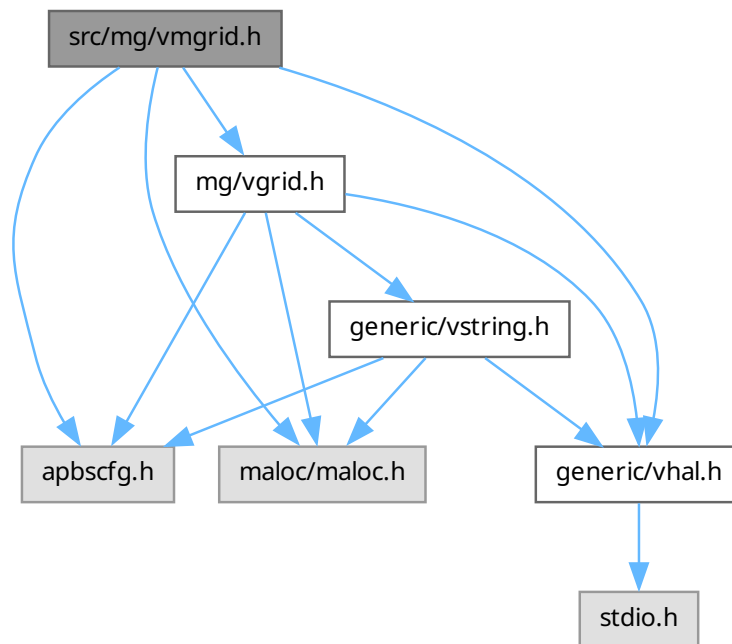
Multiresolution oracle for Cartesian mesh data.

```

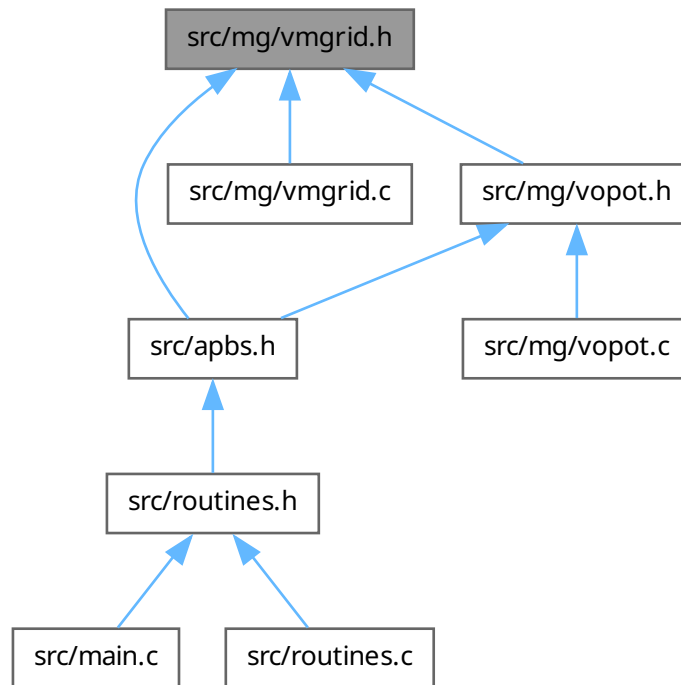
#include "apbscfg.h"
#include "maloc/maloc.h"
#include "generic/vhal.h"
#include "mg/vgrid.h"

```

Include dependency graph for vmgrid.h:



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [sVmgrid](#)
Multiresolution oracle for Cartesian mesh data.

Macros

- #define [VMGRIDMAX](#) 20
The maximum number of levels in the grid hierarchy.

Typedefs

- typedef struct [sVmgrid](#) [Vmgrid](#)
Declaration of the Vmgrid class as the Vmgrid structure.

Functions

- VEXTERNC [Vmgrid](#) * [Vmgrid_ctor](#) ()
Construct Vmgrid object.
- VEXTERNC int [Vmgrid_ctor2](#) ([Vmgrid](#) *thee)
Initialize Vmgrid object.

- VEXTERNC int [Vmgrid_value](#) ([Vmgrid](#) *thee, double x[3], double *value)
Get potential value (from mesh or approximation) at a point.
- VEXTERNC void [Vmgrid_dtor](#) ([Vmgrid](#) **thee)
Object destructor.
- VEXTERNC void [Vmgrid_dtor2](#) ([Vmgrid](#) *thee)
FORTTRAN stub object destructor.
- VEXTERNC int [Vmgrid_addGrid](#) ([Vmgrid](#) *thee, [Vgrid](#) *grid)
Add a grid to the hierarchy.
- VEXTERNC int [Vmgrid_curvature](#) ([Vmgrid](#) *thee, double pt[3], int cflag, double *curv)
Get second derivative values at a point.
- VEXTERNC int [Vmgrid_gradient](#) ([Vmgrid](#) *thee, double pt[3], double grad[3])
Get first derivative values at a point.
- VEXTERNC [Vgrid](#) * [Vmgrid_getGridByNum](#) ([Vmgrid](#) *thee, int num)
Get specific grid in hierarchy.
- VEXTERNC [Vgrid](#) * [Vmgrid_getGridByPoint](#) ([Vmgrid](#) *thee, double pt[3])
Get grid in hierarchy which contains specified point or VNULL.

9.100.1 Detailed Description

Multiresolution oracle for Cartesian mesh data.

Author

Nathan Baker

Version

\$Id\$

Attention

```
*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
* Nathan A. Baker (nathan.baker@pnnl.gov)
* Pacific Northwest National Laboratory
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*
*

```

Definition in file [vmgrid.h](#).

9.101 vmgrid.h

[Go to the documentation of this file.](#)

```

00001
00062 #ifndef _VMGRID_H_
00063 #define _VMGRID_H_
00064
00065 #include "apbscfg.h"
00066
00067 #include "malloc/malloc.h"
00068
00069 #include "generic/vhal.h"
00070 #include "mg/vgrid.h"
00071
00076 #define VMGRIDMAX 20
00077
00078
00084 struct sVmgrid {
00085     int ngrids;
00086     Vgrid *grids[VMGRIDMAX];
00092 };
00093
00098 typedef struct sVmgrid Vmgrid;
00099
00105 VEXTERNC Vmgrid* Vmgrid_ctor();
00106
00113 VEXTERNC int Vmgrid_ctor2(Vmgrid *thee);
00114
00123 VEXTERNC int Vmgrid_value(Vmgrid *thee, double x[3], double *value);
00124
00130 VEXTERNC void Vmgrid_dtor(Vmgrid **thee);
00131
00137 VEXTERNC void Vmgrid_dtor2(Vmgrid *thee);
00138
00151 VEXTERNC int Vmgrid_addGrid(Vmgrid *thee, Vgrid *grid);
00152
00153
00167 VEXTERNC int Vmgrid_curvature(Vmgrid *thee, double pt[3], int cflag,
00168     double *curv);
00169
00178 VEXTERNC int Vmgrid_gradient(Vmgrid *thee, double pt[3], double grad[3] );
00179
00187 VEXTERNC Vgrid* Vmgrid_getGridByNum(Vmgrid *thee, int num);
00188
00196 VEXTERNC Vgrid* Vmgrid_getGridByPoint(Vmgrid *thee, double pt[3]);
00197
00198 #endif
00199

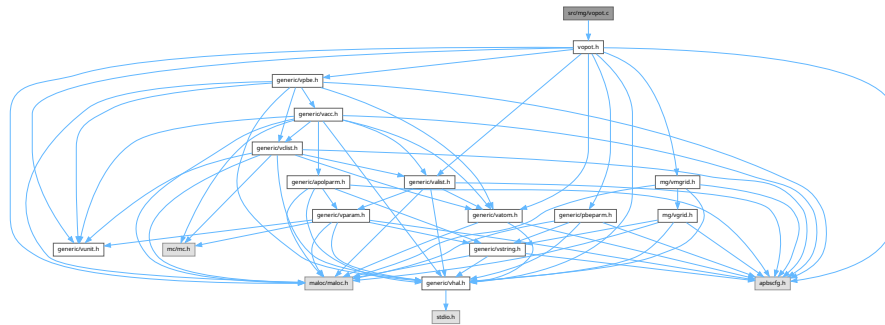
```

9.102 src/mg/vopot.c File Reference

Class Vopot methods.

```
#include "vopot.h"
```

Include dependency graph for vopot.c:



Macros

- `#define IJK(i, j, k) (((k)*(nx)*(ny))+((j)*(nx))+i)`

Functions

- `VPUBLIC Vopot * Vopot_ctor (Vmgrid *mgrid, Vpbe *pbe, Vbcfl bcfl)`
Construct Vopot object with values obtained from Vpmg_readDX (for example)
- `VPUBLIC int Vopot_ctor2 (Vopot *thee, Vmgrid *mgrid, Vpbe *pbe, Vbcfl bcfl)`
Initialize Vopot object with values obtained from Vpmg_readDX (for example)
- `VPUBLIC void Vopot_dtor (Vopot **thee)`
Object destructor.
- `VPUBLIC void Vopot_dtor2 (Vopot *thee)`
FORTTRAN stub object destructor.
- `VPUBLIC int Vopot_pot (Vopot *thee, double pt[3], double *value)`
Get potential value (from mesh or approximation) at a point.
- `VPUBLIC int Vopot_curvature (Vopot *thee, double pt[3], int cflag, double *value)`
Get second derivative values at a point.
- `VPUBLIC int Vopot_gradient (Vopot *thee, double pt[3], double grad[3])`
Get first derivative values at a point.

9.102.1 Detailed Description

Class Vopot methods.

Author

Nathan Baker

Version

\$Id\$

Attention

```

*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
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* Pacific Northwest National Laboratory
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*
*

```

Definition in file [vopot.c](#).

9.102.2 Macro Definition Documentation**9.102.2.1 IJK**

```

#define IJK(
    i,
    j,
    k ) ((k)*(nx)*(ny)) + ((j)*(nx)) + (i)

```

Definition at line 113 of file [vopot.c](#).

9.103 vopot.c

[Go to the documentation of this file.](#)

00001

```

00057 #include "vopot.h"
00058
00059 VEMBED(rcsid="$Id$")
00060
00061 /* ////////////////////////////////////////////////////////////////////
00062 // Routine: Vopot_ctor
00063 // Author: Nathan Baker
00065 VPUBLIC Vopot* Vopot_ctor(Vmgrid *mgrid, Vpbe *pbe, Vbcfl bcfl) {
00066
00067     Vopot *thee = VNULL;
00068
00069     thee = Vmem_malloc(VNULL, 1, sizeof(Vopot));
00070     VASSERT(thee != VNULL);
00071     VASSERT(Vopot_ctor2(thee, mgrid, pbe, bcfl));
00072
00073     return thee;
00074 }
00075
00076 /* ////////////////////////////////////////////////////////////////////
00077 // Routine: Vopot_ctor2
00078 // Author: Nathan Baker
00080 VPUBLIC int Vopot_ctor2(Vopot *thee, Vmgrid *mgrid, Vpbe *pbe, Vbcfl bcfl) {
00081
00082     if (thee == VNULL) return 0;
00083     thee->bcfl = bcfl;
00084     thee->mgrid = mgrid;
00085     thee->pbe = pbe;
00086
00087     return 1;
00088 }
00089
00090 /* ////////////////////////////////////////////////////////////////////
00091 // Routine: Vopot_dtor
00092 // Author: Nathan Baker
00094 VPUBLIC void Vopot_dtor(Vopot **thee) {
00095
00096     if ((*thee) != VNULL) {
00097         Vopot_dtor2(*thee);
00098         Vmem_free(VNULL, 1, sizeof(Vopot), (void **)thee);
00099         (*thee) = VNULL;
00100     }
00101 }
00102
00103 /* ////////////////////////////////////////////////////////////////////
00104 // Routine: Vopot_dtor2
00105 // Author: Nathan Baker
00107 VPUBLIC void Vopot_dtor2(Vopot *thee) { return; }
00108
00109 /* ////////////////////////////////////////////////////////////////////
00110 // Routine: Vopot_pot
00111 // Author: Nathan Baker
00113 #define IJK(i,j,k) ((k)*(nx)*(ny))+((j)*(nx))+((i))
00114 VPUBLIC int Vopot_pot(Vopot *thee, double pt[3], double *value) {
00115
00116     Vatom *atom;
00117     int i, iatom;
00118     double u, T, charge, eps_w, xkappa, dist, size, val, *position;
00119     Valist *alist;
00120
00121     VASSERT(thee != VNULL);
00122
00123     eps_w = Vpbe_getSolventDiel(thee->pbe);
00124     xkappa = (1.0e10)*Vpbe_getXkappa(thee->pbe);
00125     T = Vpbe_getTemperature(thee->pbe);
00126     alist = Vpbe_getValist(thee->pbe);
00127
00128     u = 0;
00129
00130     /* See if we're on the mesh */
00131     if (Vmgrid_value(thee->mgrid, pt, &u)) {
00132
00133         *value = u;
00134
00135     } else {
00136
00137         switch (thee->bcfl) {
00138
00139             case BCFL_ZERO:
00140                 u = 0;
00141                 break;
00142

```

```

00143     case BCFL_SDH:
00144         size = (1.0e-10)*Vpbe_getSoluteRadius(thee->pbe);
00145         position = Vpbe_getSoluteCenter(thee->pbe);
00146         charge = Vunit_ec*Vpbe_getSoluteCharge(thee->pbe);
00147         dist = 0;
00148         for (i=0; i<3; i++)
00149             dist += VSQR(position[i] - pt[i]);
00150         dist = (1.0e-10)*VSQRT(dist);
00151         val = (charge)/(4*VPI*Vunit_eps0*eps_w*dist);
00152         if (xkappa != 0.0)
00153             val = val*(exp(-xkappa*(dist-size))/(1+xkappa*size));
00154         val = val*Vunit_ec/(Vunit_kb*T);
00155         u = val;
00156         break;
00157
00158     case BCFL_MDH:
00159         u = 0;
00160         for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
00161             atom = Valist_getAtom(alist, iatom);
00162             position = Vatom_getPosition(atom);
00163             charge = Vunit_ec*Vatom_getCharge(atom);
00164             size = (1e-10)*Vatom_getRadius(atom);
00165             dist = 0;
00166             for (i=0; i<3; i++)
00167                 dist += VSQR(position[i] - pt[i]);
00168             dist = (1.0e-10)*VSQRT(dist);
00169             val = (charge)/(4*VPI*Vunit_eps0*eps_w*dist);
00170             if (xkappa != 0.0)
00171                 val = val*(exp(-xkappa*(dist-size))/(1+xkappa*size));
00172             val = val*Vunit_ec/(Vunit_kb*T);
00173             u = u + val;
00174         }
00175         break;
00176
00177     case BCFL_UNUSED:
00178         Vnm_print(2, "Vopot_pot: Invalid bcfl flag (%d)!\n",
00179             thee->bcfl);
00180         return 0;
00181
00182     case BCFL_FOCUS:
00183         Vnm_print(2, "Vopot_pot: Invalid bcfl flag (%d)!\n",
00184             thee->bcfl);
00185         return 0;
00186
00187     default:
00188         Vnm_print(2, "Vopot_pot: Bogus thee->bcfl flag (%d)!\n",
00189             thee->bcfl);
00190         return 0;
00191         break;
00192 }
00193
00194 *value = u;
00195
00196 }
00197
00198 return 1;
00199
00200 }
00201
00202 /* ////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////////
00203 // Routine: Vopot_curvature
00204 //
00205 // Notes: cflag=0 ==> Reduced Maximal Curvature
00206 //        cflag=1 ==> Mean Curvature (Laplace)
00207 //        cflag=2 ==> Gauss Curvature
00208 //        cflag=3 ==> True Maximal Curvature
00209 // If we are off the grid, we can still evaluate the Laplacian; assuming, we
00210 // are away from the molecular surface, it is simply equal to the DH factor.
00211 //
00212 // Authors: Nathan Baker
00214 VPUBLIC int Vopot_curvature(Vopot *thee, double pt[3], int cflag,
00215     double *value) {
00216
00217     Vatom *atom;
00218     int i, iatom;
00219     double u, T, charge, eps_w, xkappa, dist, size, val, *position, zkappa2;
00220     Valist *alist;
00221
00222     VASSERT(thee != VNULL);
00223
00224     eps_w = Vpbe_getSolventDiel(thee->pbe);

```

```

00225     xkappa = (1.0e10)*Vpbe_getXkappa(thee->pbe);
00226     zkappa2 = Vpbe_getZkappa2(thee->pbe);
00227     T = Vpbe_getTemperature(thee->pbe);
00228     alist = Vpbe_getValist(thee->pbe);
00229
00230     u = 0;
00231
00232     if (Vmgrid_curvature(thee->mgrid, pt, cflag, value)) return 1;
00233     else if (cflag != 1) {
00234         Vnm_print(2, "Vopot_curvature: Off mesh!\n");
00235         return 1;
00236     } else {
00237
00238         switch (thee->bcfl) {
00239
00240             case BCFL_ZERO:
00241                 u = 0;
00242                 break;
00243
00244             case BCFL_SDH:
00245                 size = (1.0e-10)*Vpbe_getSoluteRadius(thee->pbe);
00246                 position = Vpbe_getSoluteCenter(thee->pbe);
00247                 charge = Vunit_ec*Vpbe_getSoluteCharge(thee->pbe);
00248                 dist = 0;
00249                 for (i=0; i<3; i++)
00250                     dist += VSQR(position[i] - pt[i]);
00251                 dist = (1.0e-10)*VSQRT(dist);
00252                 if (xkappa != 0.0)
00253                     u = zkappa2*(exp(-xkappa*(dist-size))/(1+xkappa*size));
00254                 break;
00255
00256             case BCFL_MDH:
00257                 u = 0;
00258                 for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
00259                     atom = Valist_getAtom(alist, iatom);
00260                     position = Vatom_getPosition(atom);
00261                     charge = Vunit_ec*Vatom_getCharge(atom);
00262                     size = (1e-10)*Vatom_getRadius(atom);
00263                     dist = 0;
00264                     for (i=0; i<3; i++)
00265                         dist += VSQR(position[i] - pt[i]);
00266                     dist = (1.0e-10)*VSQRT(dist);
00267                     if (xkappa != 0.0)
00268                         val = zkappa2*(exp(-xkappa*(dist-size))/(1+xkappa*size));
00269                     u = u + val;
00270                 }
00271                 break;
00272
00273             case BCFL_UNUSED:
00274                 Vnm_print(2, "Vopot_pot: Invlid bcfl (%d)!\n", thee->bcfl);
00275                 return 0;
00276
00277             case BCFL_FOCUS:
00278                 Vnm_print(2, "Vopot_pot: Invlid bcfl (%d)!\n", thee->bcfl);
00279                 return 0;
00280
00281             default:
00282                 Vnm_print(2, "Vopot_pot: Bogus thee->bcfl flag (%d)!\n",
00283                     thee->bcfl);
00284                 return 0;
00285                 break;
00286         }
00287
00288         *value = u;
00289     }
00290
00291     return 1;
00292 }
00293
00294
00295 /* ////////////////////////////////////////
00296 // Routine: Vopot_gradient
00297 //
00298 // Authors: Nathan Baker
00300 VPUBLIC int Vopot_gradient(Vopot *thee, double pt[3], double grad[3]) {
00301
00302     Vatom *atom;
00303     int iatom;
00304     double T, charge, eps_w, xkappa, size, val, *position;
00305     double dx, dy, dz, dist;
00306     Valist *alist;

```

```

00307
00308     VASSERT(thee != VNULL);
00309
00310     eps_w = Vpbe_getSolventDiel(thee->pbe);
00311     xkappa = (1.0e10)*Vpbe_getXkappa(thee->pbe);
00312     T = Vpbe_getTemperature(thee->pbe);
00313     alist = Vpbe_getValist(thee->pbe);
00314
00315
00316     if (!Vmgrid_gradient(thee->mgrid, pt, grad)) {
00317
00318         switch (thee->bcfl) {
00319
00320             case BCFL_ZERO:
00321                 grad[0] = 0.0;
00322                 grad[1] = 0.0;
00323                 grad[2] = 0.0;
00324                 break;
00325
00326             case BCFL_SDH:
00327                 grad[0] = 0.0;
00328                 grad[1] = 0.0;
00329                 grad[2] = 0.0;
00330                 size = (1.0e-10)*Vpbe_getSoluteRadius(thee->pbe);
00331                 position = Vpbe_getSoluteCenter(thee->pbe);
00332                 charge = Vunit_ec*Vpbe_getSoluteCharge(thee->pbe);
00333                 dx = position[0] - pt[0];
00334                 dy = position[1] - pt[1];
00335                 dz = position[2] - pt[2];
00336                 dist = VSQR(dx) + VSQR(dy) + VSQR(dz);
00337                 dist = (1.0e-10)*VSQRT(dist);
00338                 val = (charge)/(4*VPI*Vunit_eps0*eps_w);
00339                 if (xkappa != 0.0)
00340                     val = val*(exp(-xkappa*(dist-size))/(1+xkappa*size));
00341                 val = val*Vunit_ec/(Vunit_kb*T);
00342                 grad[0] = val*dx/dist*(-1.0/dist/dist + xkappa/dist);
00343                 grad[1] = val*dy/dist*(-1.0/dist/dist + xkappa/dist);
00344                 grad[2] = val*dz/dist*(-1.0/dist/dist + xkappa/dist);
00345                 break;
00346
00347             case BCFL_MDH:
00348                 grad[0] = 0.0;
00349                 grad[1] = 0.0;
00350                 grad[2] = 0.0;
00351                 for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
00352                     atom = Valist_getAtom(alist, iatom);
00353                     position = Vatom_getPosition(atom);
00354                     charge = Vunit_ec*Vatom_getCharge(atom);
00355                     size = (1e-10)*Vatom_getRadius(atom);
00356                     dx = position[0] - pt[0];
00357                     dy = position[1] - pt[1];
00358                     dz = position[2] - pt[2];
00359                     dist = VSQR(dx) + VSQR(dy) + VSQR(dz);
00360                     dist = (1.0e-10)*VSQRT(dist);
00361                     val = (charge)/(4*VPI*Vunit_eps0*eps_w);
00362                     if (xkappa != 0.0)
00363                         val = val*(exp(-xkappa*(dist-size))/(1+xkappa*size));
00364                     val = val*Vunit_ec/(Vunit_kb*T);
00365                     grad[0] += (val*dx/dist*(-1.0/dist/dist + xkappa/dist));
00366                     grad[1] += (val*dy/dist*(-1.0/dist/dist + xkappa/dist));
00367                     grad[2] += (val*dz/dist*(-1.0/dist/dist + xkappa/dist));
00368                 }
00369                 break;
00370
00371             case BCFL_UNUSED:
00372                 Vnm_print(2, "Vopot: Invalid bcfl (%d)!\n", thee->bcfl);
00373                 return 0;
00374
00375             case BCFL_FOCUS:
00376                 Vnm_print(2, "Vopot: Invalid bcfl (%d)!\n", thee->bcfl);
00377                 return 0;
00378
00379             default:
00380                 Vnm_print(2, "Vopot_pot: Bogus thee->bcfl flag (%d)!\n",
00381                     thee->bcfl);
00382                 return 0;
00383                 break;
00384         }
00385
00386     return 1;
00387 }

```



```

00388
00389     return 1;
00390
00391 }

```

9.104 src/mg/vopot.h File Reference

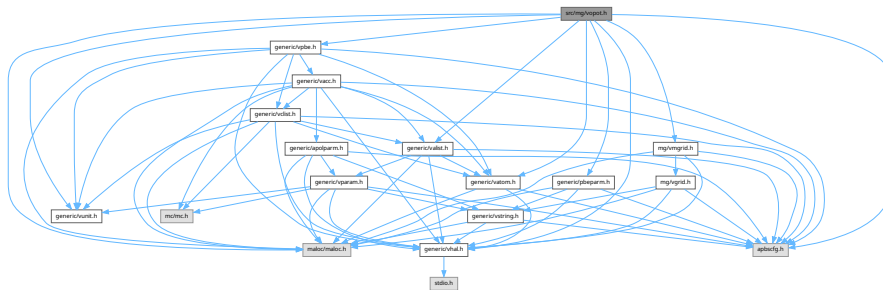
Potential oracle for Cartesian mesh data.

```

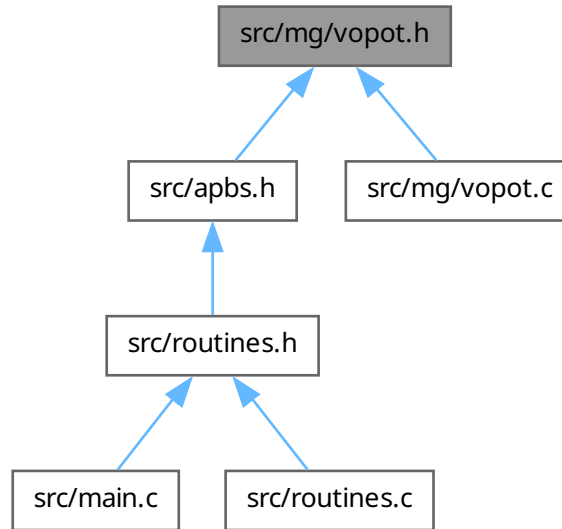
#include "apbscfg.h"
#include "malloc/malloc.h"
#include "generic/vhal.h"
#include "generic/pbeparm.h"
#include "generic/vatom.h"
#include "generic/valist.h"
#include "generic/vunit.h"
#include "generic/vpbe.h"
#include "mg/vmgrid.h"

```

Include dependency graph for vopot.h:



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [sVopot](#)
Electrostatic potential oracle for Cartesian mesh data.

Typedefs

- typedef struct [sVopot](#) [Vopot](#)
Declaration of the Vopot class as the Vopot structure.

Functions

- VEXTERNC [Vopot](#) * [Vopot_ctor](#) ([Vmgrid](#) *mgrid, [Vpbe](#) *pbe, [Vbcfl](#) bcfl)
Construct Vopot object with values obtained from Vpmg_readDX (for example)
- VEXTERNC int [Vopot_ctor2](#) ([Vopot](#) *thee, [Vmgrid](#) *mgrid, [Vpbe](#) *pbe, [Vbcfl](#) bcfl)
Initialize Vopot object with values obtained from Vpmg_readDX (for example)
- VEXTERNC int [Vopot_pot](#) ([Vopot](#) *thee, double x[3], double *pot)
Get potential value (from mesh or approximation) at a point.
- VEXTERNC void [Vopot_dtor](#) ([Vopot](#) **thee)
Object destructor.
- VEXTERNC void [Vopot_dtor2](#) ([Vopot](#) *thee)
FORTTRAN stub object destructor.
- VEXTERNC int [Vopot_curvature](#) ([Vopot](#) *thee, double pt[3], int cflag, double *curv)
Get second derivative values at a point.
- VEXTERNC int [Vopot_gradient](#) ([Vopot](#) *thee, double pt[3], double grad[3])
Get first derivative values at a point.

9.104.1 Detailed Description

Potential oracle for Cartesian mesh data.

Author

Nathan Baker

Version

\$Id\$

Attention

```
*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
* Nathan A. Baker (nathan.baker@pnnl.gov)
* Pacific Northwest National Laboratory
*
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*
*
```

Definition in file [vopot.h](#).

9.105 vopot.h

[Go to the documentation of this file.](#)

```

00001
00062 #ifndef _VOPOT_H_
00063 #define _VOPOT_H_
00064
00065 #include "apbscfg.h"
00066
00067 #include "malloc/malloc.h"
00068
00069 #include "generic/vhal.h"
00070 #include "generic/pbeparm.h"
00071 #include "generic/vatom.h"
00072 #include "generic/valist.h"
00073 #include "generic/vunit.h"
00074 #include "generic/vpbe.h"
00075 #include "generic/pbeparm.h"
00076 #include "mg/vmgrid.h"
00077
00083 struct sVopot {
00084     Vmgrid *mgrid;
00087     Vpbe *pbe;
00088     Vbcfl bcfl;
00090 };
00091
00096 typedef struct sVopot Vopot;
00097
00108 VEXTERNC Vopot* Vopot_ctor(Vmgrid *mgrid, Vpbe *pbe, Vbcfl bcfl);
00109
00121 VEXTERNC int Vopot_ctor2(Vopot *thee, Vmgrid *mgrid, Vpbe *pbe, Vbcfl bcfl);
00122
00131 VEXTERNC int Vopot_pot(Vopot *thee, double x[3], double *pot);
00132
00138 VEXTERNC void Vopot_dtor(Vopot **thee);
00139
00145 VEXTERNC void Vopot_dtor2(Vopot *thee);
00146
00160 VEXTERNC int Vopot_curvature(Vopot *thee, double pt[3], int cflag, double
00161 *curv);
00162
00171 VEXTERNC int Vopot_gradient(Vopot *thee, double pt[3], double grad[3] );
00172
00173
00174 #endif

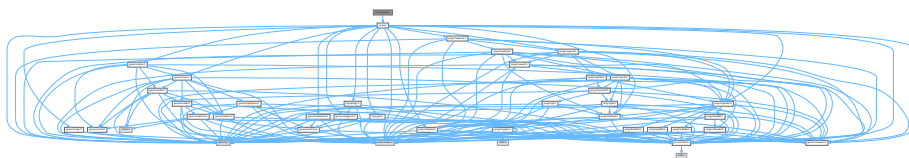
```

9.106 src/mg/vpmg.c File Reference

Class Vpmg methods.

```
#include "vpmg.h"
```

Include dependency graph for vpmg.c:



Functions

- VPUBLIC unsigned long int [Vpmg_memChk](#) ([Vpmg](#) *thee)
Return the memory used by this structure (and its contents) in bytes.
- VPUBLIC void [Vpmg_printColComp](#) ([Vpmg](#) *thee, char path[72], char title[72], char mxtype[3], int flag)
Print out a column-compressed sparse matrix in Harwell-Boeing format.
- VPUBLIC [Vpmg](#) * [Vpmg_ctor](#) ([Vpmgp](#) *pmg, [Vpbe](#) *pbe, int focusFlag, [Vpmg](#) *pmgOLD, [MGparm](#) *mgparm, [PBEparm_calcEnergy](#) energyFlag)
Constructor for the Vpmg class (allocates new memory)

- VPUBLIC int [Vpmg_ctor2](#) ([Vpmg](#) *thee, [Vpmgp](#) *pmgp, [Vpbe](#) *pbe, int focusFlag, [Vpmg](#) *pmgOLD, [MGparm](#) *mgparm, [PBEparm_calcEnergy](#) energyFlag)
FORTRAN stub constructor for the Vpmg class (uses previously-allocated memory)
- VPUBLIC int [Vpmg_solve](#) ([Vpmg](#) *thee)
Solve the PBE using PMG.
- VPUBLIC void [Vpmg_dtor](#) ([Vpmg](#) **thee)
Object destructor.
- VPUBLIC void [Vpmg_dtor2](#) ([Vpmg](#) *thee)
FORTRAN stub object destructor.
- VPUBLIC void [Vpmg_setPart](#) ([Vpmg](#) *thee, double lowerCorner[3], double upperCorner[3], int bflags[6])
Set partition information which restricts the calculation of observables to a (rectangular) subset of the problem domain.
- VPUBLIC void [Vpmg_unsetPart](#) ([Vpmg](#) *thee)
Remove partition restrictions.
- VPUBLIC int [Vpmg_fillArray](#) ([Vpmg](#) *thee, double *vec, [Vdata_Type](#) type, double parm, [Vhal_PBEType](#) pbetype, [PBEparm](#) *pbeparm)
Fill the specified array with accessibility values.
- VPRIVATE double [Vpmg_polarizEnergy](#) ([Vpmg](#) *thee, int extFlag)
Determines energy from polarizeable charge and interaction with fixed charges according to Rocchia et al.
- VPUBLIC double [Vpmg_energy](#) ([Vpmg](#) *thee, int extFlag)
Get the total electrostatic energy.
- VPUBLIC double [Vpmg_dielEnergy](#) ([Vpmg](#) *thee, int extFlag)
Get the "polarization" contribution to the electrostatic energy.
- VPUBLIC double [Vpmg_dielGradNorm](#) ([Vpmg](#) *thee)
Get the integral of the gradient of the dielectric function.
- VPUBLIC double [Vpmg_qmEnergy](#) ([Vpmg](#) *thee, int extFlag)
Get the "mobile charge" contribution to the electrostatic energy.
- VPRIVATE double [Vpmg_qmEnergyNONLIN](#) ([Vpmg](#) *thee, int extFlag)
- VPUBLIC double [Vpmg_qmEnergySMPBE](#) ([Vpmg](#) *thee, int extFlag)
Vpmg_qmEnergy for SMPBE.
- VPUBLIC double [Vpmg_qfEnergy](#) ([Vpmg](#) *thee, int extFlag)
Get the "fixed charge" contribution to the electrostatic energy.
- VPRIVATE double [Vpmg_qfEnergyPoint](#) ([Vpmg](#) *thee, int extFlag)
Calculates charge-potential energy using summation over delta function positions (i.e. something like an Linf norm)
- VPUBLIC double [Vpmg_qfAtomEnergy](#) ([Vpmg](#) *thee, [Vatom](#) *atom)
Get the per-atom "fixed charge" contribution to the electrostatic energy.
- VPRIVATE double [Vpmg_qfEnergyVolume](#) ([Vpmg](#) *thee, int extFlag)
Calculates charge-potential energy as integral over a volume.
- VPRIVATE void [Vpmg_splineSelect](#) (int srfm, [Vacc](#) *acc, double *gpos, double win, double infrad, [Vatom](#) *atom, double *force)
Selects a spline based surface method from either VSM_SPLINE, VSM_SPLINE5 or VSM_SPLINE7.
- VPRIVATE void [bcfl1](#) (double size, double *apos, double charge, double xkappa, double pre1, double *gxcf, double *gycf, double *gzcf, double *xf, double *yf, double *zf, int nx, int ny, int nz)
*Increment all boundary points by $pre1 * (charge/d) * (exp(-xkappa * (d-size)) / (1 + xkappa * size))$ to add the effect of the Debye-Huckel potential due to a single charge.*
- VPRIVATE void [bcCalcOrig](#) ([Vpmg](#) *thee)
- VPRIVATE int [gridPointsValid](#) (int i, int j, int k, int nx, int ny, int nz)
- VPRIVATE void [packAtoms](#) (double *ax, double *ay, double *az, double *charge, double *size, [Vpmg](#) *thee)

- VPRIVATE void [packUnpack](#) (int nx, int ny, int nz, int ngrid, double *gx, double *gy, double *gz, double *value, [Vpmg](#) *thee, int pack)
- VPRIVATE void [bcflnew](#) ([Vpmg](#) *thee)
- VPRIVATE void [multipolebc](#) (double r, double kappa, double eps_p, double eps_w, double rad, double tsr[3])
This routine serves bcfl2. It returns (in tsr) the contraction independent portion of the Debye-Huckel potential tensor for a spherical ion with a central charge, dipole and quadrupole. See the code for an in depth description.
- VPRIVATE void [bcfl_sdh](#) ([Vpmg](#) *thee)
- VPRIVATE void [bcfl_mdh](#) ([Vpmg](#) *thee)
- VPRIVATE void [bcfl_mem](#) (double zmem, double L, double eps_m, double eps_w, double V, double xkappa, double *gxcf, double *gycf, double *gzcf, double *xf, double *yf, double *zf, int nx, int ny, int nz)
- VPRIVATE void [bcfl_map](#) ([Vpmg](#) *thee)
- VPRIVATE void [bcCalc](#) ([Vpmg](#) *thee)
Fill boundary condition arrays.
- VPRIVATE void [fillCoCoefMap](#) ([Vpmg](#) *thee)
Fill operator coefficient arrays from pre-calculated maps.
- VPRIVATE void [fillCoCoefMol](#) ([Vpmg](#) *thee)
Fill operator coefficient arrays from a molecular surface calculation.
- VPRIVATE void [fillCoCoefMollon](#) ([Vpmg](#) *thee)
Fill ion (nonlinear) operator coefficient array from a molecular surface calculation.
- VPRIVATE void [fillCoCoefMolDiel](#) ([Vpmg](#) *thee)
Fill differential operator coefficient arrays from a molecular surface calculation.
- VPRIVATE void [fillCoCoefMolDielNoSmooth](#) ([Vpmg](#) *thee)
Fill differential operator coefficient arrays from a molecular surface calculation without smoothing.
- VPRIVATE void [fillCoCoefMolDielSmooth](#) ([Vpmg](#) *thee)
Fill differential operator coefficient arrays from a molecular surface calculation with smoothing.
- VPRIVATE void [fillCoCoefSpline](#) ([Vpmg](#) *thee)
Fill operator coefficient arrays from a spline-based surface calculation.
- VPRIVATE void [fillCoCoef](#) ([Vpmg](#) *thee)
Top-level driver to fill all operator coefficient arrays.
- VPRIVATE Vrc_Codes [fillCoCharge](#) ([Vpmg](#) *thee)
Top-level driver to fill source term charge array.
- VPRIVATE Vrc_Codes [fillCoChargeMap](#) ([Vpmg](#) *thee)
Fill source term charge array from a pre-calculated map.
- VPRIVATE void [fillCoChargeSpline1](#) ([Vpmg](#) *thee)
Fill source term charge array from linear interpolation.
- VPRIVATE double [bspline2](#) (double x)
Evaluate a cubic B-spline.
- VPRIVATE double [dbspline2](#) (double x)
Evaluate a cubic B-spline derivative.
- VPRIVATE void [fillCoChargeSpline2](#) ([Vpmg](#) *thee)
Fill source term charge array from cubic spline interpolation.
- VPUBLIC int [Vpmg_fillCo](#) ([Vpmg](#) *thee, Vsurf_Meth surfMeth, double splineWin, Vchrg_Meth chargeMeth, int useDielXMap, [Vgrid](#) *dielXMap, int useDielYMap, [Vgrid](#) *dielYMap, int useDielZMap, [Vgrid](#) *dielZMap, int useKappaMap, [Vgrid](#) *kappaMap, int usePotMap, [Vgrid](#) *potMap, int useChargeMap, [Vgrid](#) *chargeMap)
Fill the coefficient arrays prior to solving the equation.
- VPUBLIC int [Vpmg_force](#) ([Vpmg](#) *thee, double *force, int atomID, Vsurf_Meth srfrm, Vchrg_Meth chgm)
Calculate the total force on the specified atom in units of $k_B T/AA$.
- VPUBLIC int [Vpmg_ibForce](#) ([Vpmg](#) *thee, double *force, int atomID, Vsurf_Meth srfrm)

- Calculate the osmotic pressure on the specified atom in units of $k_B T/AA$.*

 - VPUBLIC int `Vpmg_dbForce` (`Vpmg *thee`, double `*dbForce`, int `atomID`, `Vsurf_Meth srfm`)
- Calculate the dielectric boundary forces on the specified atom in units of $k_B T/AA$.*

 - VPUBLIC int `Vpmg_qfForce` (`Vpmg *thee`, double `*force`, int `atomID`, `Vchrg_Meth chgm`)
- Calculate the "charge-field" force on the specified atom in units of $k_B T/AA$.*

 - VPRIVATE void `qfForceSpline1` (`Vpmg *thee`, double `*force`, int `atomID`)

Charge-field force due to a linear spline charge function.

 - VPRIVATE void `qfForceSpline2` (`Vpmg *thee`, double `*force`, int `atomID`)

Charge-field force due to a cubic spline charge function.

 - VPRIVATE void `qfForceSpline4` (`Vpmg *thee`, double `*force`, int `atomID`)

Charge-field force due to a quintic spline charge function.

 - VPRIVATE void `markFrac` (double `rtot`, double `*tpos`, int `nx`, int `ny`, int `nz`, double `hx`, double `hy`, double `hzed`, double `xmin`, double `ymin`, double `zmin`, double `*xarray`, double `*yarray`, double `*zarray`)
 - VPRIVATE void `markSphere` (double `rtot`, double `*tpos`, int `nx`, int `ny`, int `nz`, double `hx`, double `hy`, double `hz`, double `xmin`, double `ymin`, double `zmin`, double `*array`, double `markVal`)

Mark the grid points inside a sphere with a particular value. This marks by resetting the the grid points inside the sphere to the specified value.

 - VPRIVATE void `zlapSolve` (`Vpmg *thee`, double `**solution`, double `**source`, double `**work1`)

Calculate the solution to Poisson's equation with a simple Laplacian operator and zero-valued Dirichlet boundary conditions. Store the solution in `thee->u`.

 - VPUBLIC int `Vpmg_solveLaplace` (`Vpmg *thee`)

Solve Poisson's equation with a homogeneous Laplacian operator using the solvent dielectric constant. This solution is performed by a sine wave decomposition.

 - VPRIVATE double `VFCHI4` (int `i`, double `f`)

Return 2.5 plus difference of $i - f$.

 - VPRIVATE double `bspline4` (double `x`)

Evaluate a 5th Order B-Spline (4th order polynomial)

 - VPUBLIC double `db spline4` (double `x`)

Evaluate a 5th Order B-Spline derivative (4th order polynomial)

 - VPUBLIC double `d2bspline4` (double `x`)

Evaluate the 2nd derivative of a 5th Order B-Spline.

 - VPUBLIC double `d3bspline4` (double `x`)

Evaluate the 3rd derivative of a 5th Order B-Spline.

 - VPUBLIC void `fillcoPermanentMultipole` (`Vpmg *thee`)

Fill source term charge array for the use of permanent multipoles.

 - VPRIVATE void `fillcoCoefSpline4` (`Vpmg *thee`)

Fill operator coefficient arrays from a 7th order polynomial based surface calculation.

 - VPUBLIC void `fillcoPermanentInduced` (`Vpmg *thee`)
 - VPRIVATE void `fillcoCoefSpline3` (`Vpmg *thee`)

Fill operator coefficient arrays from a 5th order polynomial based surface calculation.

 - VPRIVATE void `bcolcomp` (int `*iparm`, double `*rparm`, int `*iwork`, double `*rwork`, double `*values`, int `*rowind`, int `*colptr`, int `*flag`)

Build a column-compressed matrix in Harwell-Boeing format.

 - VPRIVATE void `bcolcomp2` (int `*iparm`, double `*rparm`, int `*nx`, int `*ny`, int `*nz`, int `*iz`, int `*ipc`, double `*rpc`, double `*ac`, double `*cc`, double `*values`, int `*rowind`, int `*colptr`, int `*flag`)

Build a column-compressed matrix in Harwell-Boeing format.

 - VPRIVATE void `bcolcomp3` (int `*nx`, int `*ny`, int `*nz`, int `*ipc`, double `*rpc`, double `*ac`, double `*cc`, double `*values`, int `*rowind`, int `*colptr`, int `*flag`)

Build a column-compressed matrix in Harwell-Boeing format.

- VPRIVATE void `bcolcomp4` (int *nx, int *ny, int *nz, int *ipc, double *rpc, double *oC, double *cc, double *oE, double *oN, double *uC, double *values, int *rowind, int *colptr, int *flag)

Build a column-compressed matrix in Harwell-Boeing format.

- VPRIVATE void `pcolcomp` (int *nrow, int *ncol, int *nnzero, double *values, int *rowind, int *colptr, char *path, char *title, char *mxtype)

Print a column-compressed matrix in Harwell-Boeing format.

9.106.1 Detailed Description

Class Vpmg methods.

Author

Nathan Baker

Version

\$Id\$

Attention

```
*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
* Nathan A. Baker (nathan.baker@pnnl.gov)
* Pacific Northwest National Laboratory
*
* Additional contributing authors listed in the code documentation.
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```



```

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*
*

```

Definition in file [vpmg.c](#).

9.106.2 Function Documentation

9.106.2.1 bcCalc()

```

VPRIVATE void bcCalc (
    Vpmg * thee )

```

Fill boundary condition arrays.

Author

Nathan Baker

Definition at line [4382](#) of file [vpmg.c](#).

9.106.2.2 bcCalcOrig()

```

VPRIVATE void bcCalcOrig (
    Vpmg * thee )

```

Definition at line [2828](#) of file [vpmg.c](#).

9.106.2.3 bcfl1()

```

VPRIVATE void bcfl1 (
    double size,
    double * apos,
    double charge,
    double xkappa,
    double prel,
    double * gxcf,
    double * gycf,
    double * gzcf,
    double * xf,
    double * yf,
    double * zf,
    int nx,
    int ny,
    int nz )

```

Increment all boundary points by $\text{pre1} * (\text{charge}/d) * (\exp(-x\kappa * (d - \text{size})) / (1 + x\kappa * \text{size}))$ to add the effect of the Debye-Huckel potential due to a single charge.

Author

Nathan Baker

Parameters

<i>apos</i>	Size of the ion
<i>charge</i>	Position of the ion
<i>xkappa</i>	Charge of the ion
<i>pre1</i>	Exponential screening factor
<i>gxcf</i>	Unit- and dielectric-dependent prefactor
<i>gycf</i>	Set to x-boundary values
<i>gzcf</i>	Set to y-boundary values
<i>xf</i>	Set to z-boundary values
<i>yf</i>	Boundary point x-coordinates
<i>zf</i>	Boundary point y-coordinates
<i>nx</i>	Boundary point z-coordinates
<i>ny</i>	Number of grid points in x-direction
<i>nz</i>	Number of grid points in y-direction Number of grid points in y-direction

Definition at line [2564](#) of file [vpmg.c](#).

9.106.2.4 bcfl_map()

```
VPRIVATE void bcfl_map (
    Vpmg * thee )
```

Definition at line [4174](#) of file [vpmg.c](#).

9.106.2.5 bcfl_mdh()

```
VPRIVATE void bcfl_mdh (
    Vpmg * thee )
```

Definition at line [3868](#) of file [vpmg.c](#).

9.106.2.6 bcfl_mem()

```
VPRIVATE void bcfl_mem (
    double zmem,
    double L,
    double eps_m,
    double eps_w,
    double V,
    double xkappa,
    double * gxcf,
    double * gycf,
    double * gzcf,
    double * xf,
    double * yf,
    double * zf,
```

```

    int nx,
    int ny,
    int nz )

```

Definition at line 3995 of file [vpmg.c](#).

9.106.2.7 bcf1_sdh()

```

VPRIVATE void bcf1_sdh (
    Vpmg * thee )

```

Definition at line 3597 of file [vpmg.c](#).

9.106.2.8 bcf1new()

```

VPRIVATE void bcf1new (
    Vpmg * thee )

```

Definition at line 3407 of file [vpmg.c](#).

9.106.2.9 bspline2()

```

VPRIVATE double bspline2 (
    double x )

```

Evaluate a cubic B-spline.

Author

Nathan Baker

Returns

Cubic B-spline value

Parameters

<i>x</i>	Position
----------	----------

Definition at line 5496 of file [vpmg.c](#).

9.106.2.10 bspline4()

```

VPRIVATE double bspline4 (
    double x )

```

Evaluate a 5th Order B-Spline (4th order polynomial)

Author

: Michael Schnieders

Returns

5th Order B-Spline

Parameters

<i>x</i>	Position
----------	----------

Definition at line 7136 of file [vpmg.c](#).

9.106.2.11 d2bspline4()

```
VPUBLIC double d2bspline4 (  
    double x )
```

Evaluate the 2nd derivative of a 5th Order B-Spline.

Author

: Michael Schnieders

Returns

2nd derivative of a 5th Order B-Spline

Parameters

x	Position
---	----------

Definition at line 7202 of file [vpmg.c](#).

9.106.2.12 d3bspline4()

```
VPUBLIC double d3bspline4 (  
    double x )
```

Evaluate the 3rd derivative of a 5th Order B-Spline.

Author

: Michael Schnieders

Returns

3rd derivative of a 5th Order B-Spline

Parameters

x	Position
---	----------

Definition at line 7229 of file [vpmg.c](#).

9.106.2.13 dbspline2()

```
VPRIVATE double dbspline2 (  
    double x )
```

Evaluate a cubic B-spline derivative.

Author

Nathan Baker

Returns

Cubic B-spline derivative

Parameters

<i>x</i>	Position
----------	----------

Definition at line 5512 of file [vpmg.c](#).

9.106.2.14 db spline4()

```
VPUBLIC double db spline4 (  
    double x )
```

Evaluate a 5th Order B-Spline derivative (4th order polynomial)

Author

: Michael Schnieders

Returns

5th Order B-Spline derivative

Parameters

<i>x</i>	Position
----------	----------

Definition at line 7170 of file [vpmg.c](#).

9.106.2.15 fillcoCharge()

```
VPRIVATE Vrc_Codes fillcoCharge (  
    Vpmg * thee )
```

Top-level driver to fill source term charge array.

Returns

Success/failure status

Author

Nathan Baker

Definition at line 5287 of file [vpmg.c](#).

9.106.2.16 fillcoChargeMap()

```
VPRIVATE Vrc_Codes fillcoChargeMap (  
    Vpmg * thee )
```

Fill source term charge array from a pre-calculated map.

Returns

Success/failure status

Author

Nathan Baker

Definition at line 5343 of file [vpmg.c](#).

9.106.2.17 fillcoChargeSpline1()

```
VPRIVATE void fillcoChargeSpline1 (  
    Vpmg * thee )
```

Fill source term charge array from linear interpolation.

Author

Nathan Baker

Definition at line [5391](#) of file [vpmg.c](#).

9.106.2.18 fillcoChargeSpline2()

```
VPRIVATE void fillcoChargeSpline2 (  
    Vpmg * thee )
```

Fill source term charge array from cubic spline interpolation.

Author

Nathan Baker

Definition at line [5528](#) of file [vpmg.c](#).

9.106.2.19 fillcoCoef()

```
VPRIVATE void fillcoCoef (  
    Vpmg * thee )
```

Top-level driver to fill all operator coefficient arrays.

Author

Nathan Baker

Definition at line [5247](#) of file [vpmg.c](#).

9.106.2.20 fillcoCoefMap()

```
VPRIVATE void fillcoCoefMap (  
    Vpmg * thee )
```

Fill operator coefficient arrays from pre-calculated maps.

Author

Nathan Baker

Definition at line [4489](#) of file [vpmg.c](#).

9.106.2.21 fillcoCoefMol()

```
VPRIVATE void fillcoCoefMol (  
    Vpmg * thee )
```

Fill operator coefficient arrays from a molecular surface calculation.

Author

Nathan Baker

Definition at line [4612](#) of file [vpmg.c](#).

9.106.2.22 fillcoCoefMolDiel()

```
VPRIVATE void fillcoCoefMolDiel (  
    Vpmg * thee )
```

Fill differential operator coefficient arrays from a molecular surface calculation.

Author

Nathan Baker

Definition at line 4726 of file [vpmg.c](#).

9.106.2.23 fillcoCoefMolDielNoSmooth()

```
VPRIVATE void fillcoCoefMolDielNoSmooth (  
    Vpmg * thee )
```

Fill differential operator coefficient arrays from a molecular surface calculation without smoothing.

Author

Nathan Baker

Definition at line 4737 of file [vpmg.c](#).

9.106.2.24 fillcoCoefMolDielSmooth()

```
VPRIVATE void fillcoCoefMolDielSmooth (  
    Vpmg * thee )
```

Fill differential operator coefficient arrays from a molecular surface calculation with smoothing.

Molecular surface, dielectric smoothing following an implementation of Bruccoleri, et al. J Comput Chem 18 268-276 (1997).

This algorithm uses a 9 point harmonic smoothing technique - the point in question and all grid points 1/sqrt(2) grid spacings away.

Note

This uses thee->a1cf, thee->a2cf, thee->a3cf as temporary storage.

Author

Todd Dolinsky

Definition at line 4891 of file [vpmg.c](#).

9.106.2.25 fillcoCoefMolIon()

```
VPRIVATE void fillcoCoefMolIon (  
    Vpmg * thee )
```

Fill ion (nonlinear) operator coefficient array from a molecular surface calculation.

Author

Nathan Baker

Definition at line 4628 of file [vpmg.c](#).

9.106.2.26 fillcoCoefSpline()

```
VPRIVATE void fillcoCoefSpline (  
    Vpmg * thee )
```

Fill operator coefficient arrays from a spline-based surface calculation.

Author

Nathan Baker

Definition at line 5022 of file [vpmg.c](#).

9.106.2.27 fillcoCoefSpline3()

```
VPRIVATE void fillcoCoefSpline3 (  
    Vpmg * thee )
```

Fill operator coefficient arrays from a 5th order polynomial based surface calculation.

Author

Michael Schnieders

Definition at line 10430 of file [vpmg.c](#).

9.106.2.28 fillcoCoefSpline4()

```
VPRIVATE void fillcoCoefSpline4 (  
    Vpmg * thee )
```

Fill operator coefficient arrays from a 7th order polynomial based surface calculation.

Author

Michael Schnieders

Definition at line 9939 of file [vpmg.c](#).

9.106.2.29 fillcoPermanentInduced()

```
VPUBLIC void fillcoPermanentInduced (  
    Vpmg * thee )
```

Definition at line 10260 of file [vpmg.c](#).

9.106.2.30 fillcoPermanentMultipole()

```
VPUBLIC void fillcoPermanentMultipole (  
    Vpmg * thee )
```

Fill source term charge array for the use of permanent multipoles.

Author

Michael Schnieders

Definition at line 7240 of file [vpmg.c](#).

9.106.2.31 gridPointIsValid()

```
VPRIVATE int gridPointIsValid (  
    int i,  
    int j,  
    int k,
```



```

    int nx,
    int ny,
    int nz )

```

Definition at line 3130 of file [vpmg.c](#).

9.106.2.32 markFrac()

```

VPRIVATE void markFrac (
    double rtot,
    double * tpos,
    int nx,
    int ny,
    int nz,
    double hx,
    double hy,
    double hzed,
    double xmin,
    double ymin,
    double zmin,
    double * xarray,
    double * yarray,
    double * zarray )

```

Definition at line 6684 of file [vpmg.c](#).

9.106.2.33 markSphere()

```

VPRIVATE void markSphere (
    double rtot,
    double * tpos,
    int nx,
    int ny,
    int nz,
    double hx,
    double hy,
    double hzed,
    double xmin,
    double ymin,
    double zmin,
    double * array,
    double markVal )

```

Mark the grid points inside a sphere with a particular value. This marks by resetting the the grid points inside the sphere to the specified value.

Author

Nathan Baker

Parameters

<i>tpos</i>	Sphere radius
<i>nx</i>	Sphere position
<i>ny</i>	Number of grid points
<i>nz</i>	Number of grid points
<i>hx</i>	Number of grid points

Parameters

<i>hy</i>	Grid spacing
<i>hz</i>	Grid spacing
<i>xmin</i>	Grid spacing
<i>ymin</i>	Grid lower corner
<i>zmin</i>	Grid lower corner
<i>array</i>	Grid lower corner
<i>markVal</i>	Grid values Value to mark with

Definition at line 6849 of file [vpmg.c](#).

9.106.2.34 multipolebc()

```
VPRIVATE void multipolebc (
    double r,
    double kappa,
    double eps_p,
    double eps_w,
    double rad,
    double tsr[3] )
```

This routine serves bcf12. It returns (in tsr) the contraction independent portion of the Debye-Huckel potential tensor for a spherical ion with a central charge, dipole and quadrupole. See the code for an in depth description.

Author

Michael Schnieders

Parameters

<i>kappa</i>	Distance to the boundary
<i>eps</i> ↔ <i>_p</i>	Exponential screening factor
<i>eps</i> ↔ <i>_w</i>	Solute dielectric
<i>rad</i>	Solvent dielectric
<i>tsr</i>	Radius of the sphere Contraction-independent portion of each tensor

Definition at line 3487 of file [vpmg.c](#).

9.106.2.35 packAtoms()

```
VPRIVATE void packAtoms (
    double * ax,
    double * ay,
    double * az,
    double * charge,
    double * size,
    Vpmg * thee )
```

Definition at line 3313 of file [vpmg.c](#).

9.106.2.36 packUnpack()

```
VPRIVATE void packUnpack (
    int nx,
    int ny,
    int nz,
    int ngrid,
    double * gx,
    double * gy,
    double * gz,
    double * value,
    Vpmg * thee,
    int pack )
```

Definition at line 3338 of file [vpmg.c](#).

9.106.2.37 qfForceSpline1()

```
VPRIVATE void qfForceSpline1 (
    Vpmg * thee,
    double * force,
    int atomID )
```

Charge-field force due to a linear spline charge function.

Author

Nathan Baker

Parameters

<i>atomID</i>	Set to force Valist atom ID
---------------	-----------------------------

Definition at line 6311 of file [vpmg.c](#).

9.106.2.38 qfForceSpline2()

```
VPRIVATE void qfForceSpline2 (
    Vpmg * thee,
    double * force,
    int atomID )
```

Charge-field force due to a cubic spline charge function.

Author

Nathan Baker

Parameters

<i>atomID</i>	Set to force Valist atom ID
---------------	-----------------------------

Definition at line 6448 of file [vpmg.c](#).

9.106.2.39 qfForceSpline4()

```
VPRIVATE void qfForceSpline4 (
    Vpmg * thee,
```

```
double * force,
int atomID )
```

Charge-field force due to a quintic spline charge function.

Author

Michael Schnieders

Parameters

<i>atomID</i>	Set to force Valist atom ID
---------------	-----------------------------

Definition at line [6561](#) of file [vpmg.c](#).

9.106.2.40 VFCHI4()

```
VPRIVATE double VFCHI4 (
    int i,
    double f )
```

Return 2.5 plus difference of i - f.

Author

Michael Schnieders

Returns

(2.5+((double)(i)-(f)))

Definition at line [7132](#) of file [vpmg.c](#).

9.106.2.41 Vpmg_polarizEnergy()

```
VPRIVATE double Vpmg_polarizEnergy (
    Vpmg * thee,
    int extFlag )
```

Determines energy from polarizeable charge and interaction with fixed charges according to Rocchia et al.

Author

Nathan Baker

Returns

Energy in kT

Parameters

<i>extFlag</i>	If 1, add external energy contributions to result
----------------	---

Definition at line [1148](#) of file [vpmg.c](#).

9.106.2.42 Vpmg_qfEnergyPoint()

```
VPRIVATE double Vpmg_qfEnergyPoint (
    Vpmg * thee,
```

```
int extFlag )
```

Calculates charge-potential energy using summation over delta function positions (i.e. something like an Linf norm)

Author

Nathan Baker

Returns

Energy in kT

Parameters

<i>extFlag</i>	If 1, add external energy contributions to result
----------------	---

Definition at line 1704 of file [vpmg.c](#).

9.106.2.43 Vpmg_qfEnergyVolume()

```
VPRIVATE double Vpmg_qfEnergyVolume (
    Vpmg * thee,
    int extFlag )
```

Calculates charge-potential energy as integral over a volume.

Author

Nathan Baker

Returns

Energy in kT

Parameters

<i>extFlag</i>	If 1, add external energy contributions to result
----------------	---

Definition at line 1861 of file [vpmg.c](#).

9.106.2.44 Vpmg_qmEnergyNONLIN()

```
VPRIVATE double Vpmg_qmEnergyNONLIN (
    Vpmg * thee,
    int extFlag )
```

Definition at line 1401 of file [vpmg.c](#).

9.106.2.45 Vpmg_qmEnergySMPBE()

```
VPUBLIC double Vpmg_qmEnergySMPBE (
    Vpmg * thee,
    int extFlag )
```

Vpmg_qmEnergy for SMPBE.

Author

Vincent Chu

Definition at line 1490 of file [vpmg.c](#).

9.106.2.46 Vpmg_splineSelect()

```
VPRIVATE void Vpmg_splineSelect (
    int srfm,
    Vacc * acc,
    double * gpos,
    double win,
    double infrad,
    Vatom * atom,
    double * force )
```

Selects a spline based surface method from either VSM_SPLINE, VSM_SPLINE5 or VSM_SPLINE7.

Author

David Gohara

Parameters

<i>acc</i>	Surface method, currently VSM_SPLINE, VSM_SPLINE5, or VSM_SPLINE7
<i>gpos</i>	Accessibility object
<i>win</i>	Position array -> array[3]
<i>infrad</i>	Spline window
<i>atom</i>	Inflation radius
<i>force</i>	Atom object Force array -> array[3]

Definition at line 1893 of file [vpmg.c](#).

9.106.2.47 zlapSolve()

```
VPRIVATE void zlapSolve (
    Vpmg * thee,
    double ** solution,
    double ** source,
    double ** work1 )
```

Calculate the solution to Poisson's equation with a simple Laplacian operator and zero-valued Dirichlet boundary conditions. Store the solution in *thee*->u.

Author

Nathan Baker

Note

Vpmg_fillco must be called first

Parameters

<i>source</i>	Solution term vector
<i>work1</i>	Source term vector Work vector

Definition at line 6898 of file [vpmg.c](#).

9.107 vpmg.c

[Go to the documentation of this file.](#)

```

00001
00073 #include "vpmg.h"
00074
00075 VEMBED(rcsid="$Id$")
00076
00077 #if !defined(VINLINE_VPMG)
00078
00079 VPUBLIC unsigned long int Vpmg_memChk(Vpmg *thee) {
00080     if (thee == VNULL) return 0;
00081     return Vmem_bytes(thee->vmem);
00082 }
00083
00084 #endif /* if !defined(VINLINE_VPMG) */
00085
00086
00087 VPUBLIC void Vpmg_printColComp(Vpmg *thee, char path[72], char title[72],
00088     char mxtype[3], int flag) {
00089
00090     int nn, nxm2, nym2, nzm2, ncol, nrow, nonz;
00091     double *nzval;
00092     int *colptr, *rowind;
00093
00094     /* Calculate the total number of unknowns */
00095     nxm2 = thee->pmgp->nx - 2;
00096     nym2 = thee->pmgp->ny - 2;
00097     nzm2 = thee->pmgp->nz - 2;
00098     nn = nxm2*ny + nzm2;
00099     ncol = nn;
00100     nrow = nn;
00101
00102     /* Calculate the number of non-zero matrix entries:
00103     *   nn      nonzeros on diagonal
00104     *   nn-1    nonzeros on first off-diagonal
00105     *   nn-nx   nonzeros on second off-diagonal
00106     *   nn-nx*ny nonzeros on third off-diagonal
00107     *
00108     *   7*nn-2*nx*ny-2*nx-2 TOTAL non-zeros
00109     */
00110     nonz = 7*nn - 2*nxm2*ny + 2*nxm2 - 2;
00111     nzval = (double*)Vmem_malloc(thee->vmem, nonz, sizeof(double));
00112     rowind = (int*)Vmem_malloc(thee->vmem, nonz, sizeof(int));
00113     colptr = (int*)Vmem_malloc(thee->vmem, (ncol+1), sizeof(int));
00114
00115     #ifndef VAPBSQUIET
00116     Vnm_print(1, "Vpmg_printColComp: Allocated space for %d nonzeros\n",
00117         nonz);
00118     #endif
00119
00120     bcolcomp(thee->iparm, thee->rparm, thee->iwork, thee->rwork,
00121         nzval, rowind, colptr, &flag);
00122
00123
00124     #if 0
00125     for (i=0; i<nn; i++) {
00126         Vnm_print(1, "nnz(%d) = %g\n", i, nzval[i]);
00127     }
00128     #endif
00129
00130     /* I do not understand why I need to pass nzval in this way, but it
00131     * works... */
00132     pcolcomp(&nrow, &ncol, &nonz, &(nzval[0]), rowind, colptr, path, title,
00133         mxtype);
00134
00135     Vmem_free(thee->vmem, (ncol+1), sizeof(int), (void **)&colptr);
00136     Vmem_free(thee->vmem, nonz, sizeof(int), (void **)&rowind);
00137     Vmem_free(thee->vmem, nonz, sizeof(double), (void **)&nzval);
00138
00139 }
00140
00141 VPUBLIC Vpmg* Vpmg_ctor(Vpmgp *pmgp, Vpbe *pbe, int focusFlag,
00142     Vpmg *pmgOLD, MGparm *mgparm, PBEparm_calcEnergy energyFlag) {
00143
00144     Vpmg *thee = VNULL;
00145
00146     thee = (Vpmg*)Vmem_malloc(VNULL, 1, sizeof(Vpmg));
00147     VASSERT(thee != VNULL);
00148     VASSERT( Vpmg_ctor2(thee, pmgp, pbe, focusFlag, pmgOLD, mgparm,

```

```

00149         energyFlag) );
00150     return thee;
00151 }
00152
00153 VPUBLIC int Vpmg_ctor2(Vpmg *thee, Vpmgp *pmgp, Vpbe *pbe, int focusFlag,
00154                      Vpmg *pmgOLD, MGparm *mgparm, PBEparm_calcEnergy energyFlag) {
00155     int i, j, nion;
00156     double ionConc[MAXION], ionQ[MAXION], ionRadii[MAXION], zkappa2, zks2;
00157     double ionstr, partMin[3], partMax[3];
00158     size_t size;
00159
00160     /* Get the parameters */
00161     VASSERT(pmgp != VNULL);
00162     VASSERT(pbe != VNULL);
00163     thee->pmgp = pmgp;
00164     thee->pbe = pbe;
00165
00166     /* Set up the memory */
00167     thee->vmem = Vmem_ctor("APBS:VPMG");
00168
00169     /* Initialize ion concentrations and valencies in PMG routines */
00170     zkappa2 = Vpbe_getZkappa2(thee->pbe);
00171     ionstr = Vpbe_getBulkIonicStrength(thee->pbe);
00172     if (ionstr > 0.0) zks2 = 0.5/ionstr;
00173     else zks2 = 0.0;
00174     Vpbe_getIons(thee->pbe, &nion, ionConc, ionRadii, ionQ);
00175
00176     /* TEMPORARY USEAQUA */
00177     /* Calculate storage requirements */
00178     if (mgparm->useAqua == 0){
00179         Vpmgp_size(thee->pmgp);
00180     }else{
00181         VABORT_MSG0("Aqua is currently disabled");
00182     }
00183
00184     /* We need some additional storage if: nonlinear & newton OR cgm */
00185     /* SMPBE Added - nonlin = 2 added since it mimics NPBE */
00186     if ( ( (thee->pmgp->nonlin == NONLIN_NPBE) || (thee->pmgp->nonlin == NONLIN_SMPBE))
00187         && (thee->pmgp->meth == VSOL_Newton) ) || (thee->pmgp->meth == VSOL_CGM) )
00188     {
00189         thee->pmgp->nrvk += (2*(thee->pmgp->nf));
00190     }
00191
00192     if (thee->pmgp->iinfo > 1) {
00193         Vnm_print(2, "Vpmg_ctor2: PMG chose nx = %d, ny = %d, nz = %d\n",
00194                 thee->pmgp->nx, thee->pmgp->ny, thee->pmgp->nz);
00195         Vnm_print(2, "Vpmg_ctor2: PMG chose nlev = %d\n",
00196                 thee->pmgp->nlev);
00197         Vnm_print(2, "Vpmg_ctor2: PMG chose nxc = %d, nyc = %d, nzc = %d\n",
00198                 thee->pmgp->nxc, thee->pmgp->nyc, thee->pmgp->nzc);
00199         Vnm_print(2, "Vpmg_ctor2: PMG chose nf = %d, nc = %d\n",
00200                 thee->pmgp->nf, thee->pmgp->nc);
00201         Vnm_print(2, "Vpmg_ctor2: PMG chose narr = %d, narrc = %d\n",
00202                 thee->pmgp->narr, thee->pmgp->narrc);
00203         Vnm_print(2, "Vpmg_ctor2: PMG chose n_rpc = %d, n_iz = %d, n_ipc = %d\n",
00204                 thee->pmgp->n_rpc, thee->pmgp->n_iz, thee->pmgp->n_ipc);
00205         Vnm_print(2, "Vpmg_ctor2: PMG chose nrwk = %d, niwk = %d\n",
00206                 thee->pmgp->nrwk, thee->pmgp->niwk);
00207     }
00208
00209     /* Allocate boundary storage */
00210     thee->gxcf = (double *)Vmem_malloc(
00211         thee->vmem,
00212         10*(thee->pmgp->ny)*(thee->pmgp->nz),
00213         sizeof(double)
00214     );
00215
00216     thee->gycf = (double *)Vmem_malloc(
00217         thee->vmem,
00218         10*(thee->pmgp->nx)*(thee->pmgp->nz),
00219         sizeof(double)
00220     );
00221
00222     thee->gzcf = (double *)Vmem_malloc(
00223         thee->vmem,

```



```

00231         10*(thee->pmgp->nx)*(thee->pmgp->ny),
00232         sizeof(double)
00233     );
00234
00235
00236
00237     /* Warn users if they are using BCFL_MAP that
00238        we do not include external energies */
00239     if (thee->pmgp->bcfl == BCFL_MAP)
00240         Vnm_print(2, "Vpmg_ctor2: \nWarning: External energies are not used in BCFL_MAP calculations!\n");
00241
00242     if (focusFlag) {
00243
00244         /* Overwrite any default or user-specified boundary condition
00245            * arguments; we are now committed to a calculation via focusing */
00246         if (thee->pmgp->bcfl != BCFL_FOCUS) {
00247             Vnm_print(2,
00248                 "Vpmg_ctor2: reset boundary condition flag to BCFL_FOCUS!\n");
00249             thee->pmgp->bcfl = BCFL_FOCUS;
00250         }
00251
00252         /* Fill boundaries */
00253         Vnm_print(0, "Vpmg_ctor2: Filling boundary with old solution!\n");
00254         focusFillBound(thee, pmgOLD);
00255
00256         /* Calculate energetic contributions from region outside focusing
00257            * domain */
00258         if (energyFlag != PCE_NO) {
00259
00260             if (mgparm->type == MCT_PARALLEL) {
00261
00262                 for (j=0; j<3; j++) {
00263                     partMin[j] = mgparm->partDisjCenter[j]
00264                         - 0.5*mgparm->partDisjLength[j];
00265                     partMax[j] = mgparm->partDisjCenter[j]
00266                         + 0.5*mgparm->partDisjLength[j];
00267                 }
00268
00269                 } else {
00270                     for (j=0; j<3; j++) {
00271                         partMin[j] = mgparm->center[j] - 0.5*mgparm->glen[j];
00272                         partMax[j] = mgparm->center[j] + 0.5*mgparm->glen[j];
00273                     }
00274                 }
00275                 extEnergy(thee, pmgOLD, energyFlag, partMin, partMax,
00276                     mgparm->partDisjOwnSide);
00277             }
00278
00279         } else {
00280
00281             /* Ignore external energy contributions */
00282             thee->extQmEnergy = 0;
00283             thee->extDiEnergy = 0;
00284             thee->extQfEnergy = 0;
00285         }
00286
00287         /* Allocate partition vector storage */
00288         size = (thee->pmgp->nx)*(thee->pmgp->ny)*(thee->pmgp->nz);
00289         thee->pvec = (double *)Vmem_malloc(
00290             thee->vmem,
00291             size,
00292             sizeof(double)
00293         );
00294
00295         /* Allocate remaining storage */
00296         thee->iparm = (int *)Vmem_malloc(thee->vmem, 100, sizeof(int));
00297         thee->rparm = (double *)Vmem_malloc(thee->vmem, 100, sizeof(double));
00298         thee->iwork = (int *)Vmem_malloc(thee->vmem, thee->pmgp->niwk, sizeof(int));
00299         thee->rwork = (double *)Vmem_malloc(thee->vmem, thee->pmgp->nrwk, sizeof(double));
00300         thee->charge = (double *)Vmem_malloc(thee->vmem, thee->pmgp->narr, sizeof(double));
00301         thee->kappa = (double *)Vmem_malloc(thee->vmem, thee->pmgp->narr, sizeof(double));
00302         thee->pot = (double *)Vmem_malloc(thee->vmem, thee->pmgp->narr, sizeof(double));
00303         thee->epsx = (double *)Vmem_malloc(thee->vmem, thee->pmgp->narr, sizeof(double));
00304         thee->epsy = (double *)Vmem_malloc(thee->vmem, thee->pmgp->narr, sizeof(double));
00305         thee->epsz = (double *)Vmem_malloc(thee->vmem, thee->pmgp->narr, sizeof(double));
00306         thee->alcf = (double *)Vmem_malloc(thee->vmem, thee->pmgp->narr, sizeof(double));
00307         thee->a2cf = (double *)Vmem_malloc(thee->vmem, thee->pmgp->narr, sizeof(double));
00308         thee->a3cf = (double *)Vmem_malloc(thee->vmem, thee->pmgp->narr, sizeof(double));
00309         thee->ccf = (double *)Vmem_malloc(thee->vmem, thee->pmgp->narr, sizeof(double));
00310         thee->fcf = (double *)Vmem_malloc(thee->vmem, thee->pmgp->narr, sizeof(double));
00311         thee->tcf = (double *)Vmem_malloc(thee->vmem, thee->pmgp->narr, sizeof(double));

```

```

00312     thee->u      = (double *)Vmem_malloc(thee->vmem,  thee->pmgp->narr,  sizeof(double));
00313     thee->xf      = (double *)Vmem_malloc(thee->vmem,  5*(thee->pmgp->nx),  sizeof(double));
00314     thee->yf      = (double *)Vmem_malloc(thee->vmem,  5*(thee->pmgp->ny),  sizeof(double));
00315     thee->zf      = (double *)Vmem_malloc(thee->vmem,  5*(thee->pmgp->nz),  sizeof(double));
00316
00317
00318
00319     /* Packs parameters into the iparm and rparm arrays */
00320     Vpackmg(thee->iparm, thee->rparm, &(thee->pmgp->nrvk), &(thee->pmgp->niwk),
00321             &(thee->pmgp->nx), &(thee->pmgp->ny), &(thee->pmgp->nz),
00322             &(thee->pmgp->nlev), &(thee->pmgp->nul1), &(thee->pmgp->nu2),
00323             &(thee->pmgp->mgkey), &(thee->pmgp->itmax), &(thee->pmgp->istop),
00324             &(thee->pmgp->ipcon), &(thee->pmgp->nonlin), &(thee->pmgp->mgsmoo),
00325             &(thee->pmgp->mgprol), &(thee->pmgp->mgcoar), &(thee->pmgp->mgslv),
00326             &(thee->pmgp->mgdisc), &(thee->pmgp->iinfo), &(thee->pmgp->errtol),
00327             &(thee->pmgp->ipkey), &(thee->pmgp->omegal), &(thee->pmgp->omegan),
00328             &(thee->pmgp->irite), &(thee->pmgp->iperf));
00329
00330
00331
00332     /* Currently for SMPBE type calculations we do not want to apply a scale
00333        factor to the ionConc */
00334     switch(pmgp->ipkey){
00341
00342         case IPKEY_SMPBE:
00343
00344             Vmypdefinitmpbe(&nion, ionQ, ionConc, &pbe->smvolume, &pbe->smsize);
00345
00346             break;
00347
00348
00349         case IPKEY_NPBE:
00350
00351             /* Else adjust the ionConc by scaling factor zks2 */
00352             for (i=0; i<nion; i++)
00353                 ionConc[i] = zks2 * ionConc[i];
00354
00355             Vmypdefinitnpbe(&nion, ionQ, ionConc);
00356
00357             break;
00358
00359
00360         case IPKEY_LPBE:
00361
00362             /* Else adjust the ionConc by scaling factor zks2 */
00363             for (i=0; i<nion; i++)
00364                 ionConc[i] = zks2 * ionConc[i];
00365
00366             Vmypdefinitlpbe(&nion, ionQ, ionConc);
00367
00368             break;
00369
00370
00371         default:
00372             Vnm_print(2, "PMG: Warning: PBE structure not initialized!\n");
00373             /* Else adjust the ionConc by scaling factor zks2 */
00374             for (i=0; i<nion; i++)
00375                 ionConc[i] = zks2 * ionConc[i];
00376
00377             break;
00378     }
00379
00380     /* Set the default chargeSrc for 5th order splines */
00381     thee->chargeSrc = mgparm->chgs;
00382
00383     /* Turn off restriction of observable calculations to a specific
00384        * partition */
00385     Vpmg_unsetPart(thee);
00386
00387     /* The coefficient arrays have not been filled */
00388     thee->filled = 0;
00389
00390
00391     /*
00392      * TODO: Move the dtor out of here. The current ctor is done in routines.c,
00393      *       This was originally moved out to kill a memory leak. The dtor has
00394      *       has been removed from initMG and placed back here to keep memory
00395      *       usage low. killMG has been modified accordingly.
00396      */
00397     Vpmg_dtor(&pmgOLD);
00398
00399     return 1;

```

```

00399 }
00400
00401 VPUBLIC int Vpmg_solve(Vpmg *thee) {
00402     int i,
00403         nx,
00404         ny,
00405         nz,
00406         n;
00407     double zkappa2;
00408
00409     nx = thee->pmgp->nx;
00410     ny = thee->pmgp->ny;
00411     nz = thee->pmgp->nz;
00412     n = nx*ny*nz;
00413
00414     if (!(thee->filled)) {
00415         Vnm_print(2, "Vpmg_solve: Need to call Vpmg_fillco()!\n");
00416         return 0;
00417     }
00418
00419     /* Fill the "true solution" array */
00420     for (i=0; i<n; i++) {
00421         thee->tcf[i] = 0.0;
00422     }
00423
00424     /* Fill the RHS array */
00425     for (i=0; i<n; i++) {
00426         thee->fcf[i] = thee->charge[i];
00427     }
00428
00429     /* Fill the operator coefficient array. */
00430     for (i=0; i<n; i++) {
00431         thee->alcf[i] = thee->epsx[i];
00432         thee->a2cf[i] = thee->epsy[i];
00433         thee->a3cf[i] = thee->epsz[i];
00434     }
00435
00436     /* Fill the nonlinear coefficient array by multiplying the kappa
00437      * accessibility array (containing values between 0 and 1) by zkappa2. */
00438     zkappa2 = Vpbe_getZkappa2(thee->pbe);
00439     if (zkappa2 > VPMGSMALL) {
00440         for (i=0; i<n; i++) {
00441             thee->ccf[i] = zkappa2*thee->kappa[i];
00442         }
00443     } else {
00444         for (i=0; i<n; i++) {
00445             thee->ccf[i] = 0.0;
00446         }
00447     }
00448
00449     switch(thee->pmgp->meth) {
00450         /* CGMG (linear) */
00451         case VSOL_CGMG:
00452             if (thee->pmgp->iinfo > 1)
00453                 Vnm_print(2, "Driving with CGMGDRIV\n");
00454             VABORT_MSG0("CGMGDRIV is not currently supported");
00455             break;
00456
00457         /* Newton (nonlinear) */
00458         case VSOL_Newton:
00459             if (thee->pmgp->iinfo > 1)
00460                 Vnm_print(2, "Driving with NEWDRIV\n");
00461             Vnewdriv
00462                 (thee->iparm, thee->rparm, thee->iwork, thee->rwork,
00463                  thee->u, thee->xf, thee->yf, thee->zf, thee->gxcf, thee->gycf,
00464                  thee->gzcf, thee->alcf, thee->a2cf, thee->a3cf, thee->ccf,
00465                  thee->fcf, thee->tcf);
00466             break;
00467
00468         /* MG (linear/nonlinear) */
00469         case VSOL_MG:
00470             if (thee->pmgp->iinfo > 1)
00471                 Vnm_print(2, "Driving with MGDIV\n");
00472             Vmgdriv(thee->iparm, thee->rparm, thee->iwork, thee->rwork,

```

```

00480                                     thee->u, thee->xf, thee->yf, thee->zf, thee->gxcf, thee->gycf,
00481                                     thee->gzcf, thee->a1cf, thee->a2cf, thee->a3cf, thee->ccf,
00482                                     thee->fcf, thee->tcf);
00483     break;
00484
00485     /* CGHS (linear/nonlinear) */
00486     case VSOL_CG:
00487
00488         if (thee->pmgp->iinfo > 1)
00489             Vnm_print(2, "Driving with NCGHSDRIV\n");
00490
00491         VABORT_MSG0("NCGHSDRIV is not currently supported");
00492         break;
00493
00494     /* SOR (linear/nonlinear) */
00495     case VSOL_SOR:
00496
00497         if (thee->pmgp->iinfo > 1)
00498             Vnm_print(2, "Driving with NSORDRIV\n");
00499
00500         VABORT_MSG0("NSORDRIV is not currently supported");
00501         break;
00502
00503     /* GSRB (linear/nonlinear) */
00504     case VSOL_RBGS:
00505
00506         if (thee->pmgp->iinfo > 1)
00507             Vnm_print(2, "Driving with NGSRBDRIV\n");
00508
00509         VABORT_MSG0("NGSRBDRIV is not currently supported");
00510         break;
00511
00512     /* WJAC (linear/nonlinear) */
00513     case VSOL_WJ:
00514
00515         if (thee->pmgp->iinfo > 1)
00516             Vnm_print(2, "Driving with NWJACDRIV\n");
00517
00518         VABORT_MSG0("NWJACDRIV is not currently supported");
00519         break;
00520
00521     /* RICH (linear/nonlinear) */
00522     case VSOL_Richardson:
00523
00524         if (thee->pmgp->iinfo > 1)
00525             Vnm_print(2, "Driving with NRICHDRIV\n");
00526
00527         VABORT_MSG0("NRICHDRIV is not currently supported");
00528         break;
00529
00530     /* CGMG (linear) TEMPORARY USEAQUA */
00531     case VSOL_CGMGAqua:
00532
00533         if (thee->pmgp->iinfo > 1)
00534             Vnm_print(2, "Driving with CGMGDRIVAQUA\n");
00535
00536         VABORT_MSG0("CGMGDRIVAQUA is not currently supported");
00537         break;
00538
00539     /* Newton (nonlinear) TEMPORARY USEAQUA */
00540     case VSOL_NewtonAqua:
00541
00542         if (thee->pmgp->iinfo > 1)
00543             Vnm_print(2, "Driving with NEWDRIVAQUA\n");
00544
00545         VABORT_MSG0("NEWDRIVAQUA is not currently supported");
00546         break;
00547
00548     /* Error handling */
00549     default:
00550         Vnm_print(2, "Vpmg_solve: invalid solver method key (%d)\n",
00551                 thee->pmgp->key);
00552         return 0;
00553         break;
00554 }
00555
00556 return 1;
00557
00558 }
00559
00560

```

```

00561 VPUBLIC void Vpmg_dtor(Vpmg **thee) {
00562
00563     if ((*thee) != VNULL) {
00564         Vpmg_dtor2(*thee);
00565         Vmem_free(VNULL, 1, sizeof(Vpmg), (void **)thee);
00566         (*thee) = VNULL;
00567     }
00568
00569 }
00570
00571 VPUBLIC void Vpmg_dtor2(Vpmg *thee) {
00572
00573     /* Clean up the storage */
00574
00575     Vmem_free(thee->vmem, 100, sizeof(int),
00576         (void *)&(thee->iparm));
00577     Vmem_free(thee->vmem, 100, sizeof(double),
00578         (void *)&(thee->rparm));
00579     Vmem_free(thee->vmem, thee->pmgp->niwk, sizeof(int),
00580         (void *)&(thee->iwork));
00581     Vmem_free(thee->vmem, thee->pmgp->nrwk, sizeof(double),
00582         (void *)&(thee->rwork));
00583     Vmem_free(thee->vmem, thee->pmgp->narr, sizeof(double),
00584         (void *)&(thee->charge));
00585     Vmem_free(thee->vmem, thee->pmgp->narr, sizeof(double),
00586         (void *)&(thee->kappa));
00587     Vmem_free(thee->vmem, thee->pmgp->narr, sizeof(double),
00588         (void *)&(thee->pot));
00589     Vmem_free(thee->vmem, thee->pmgp->narr, sizeof(double),
00590         (void *)&(thee->epsx));
00591     Vmem_free(thee->vmem, thee->pmgp->narr, sizeof(double),
00592         (void *)&(thee->epsy));
00593     Vmem_free(thee->vmem, thee->pmgp->narr, sizeof(double),
00594         (void *)&(thee->epsz));
00595     Vmem_free(thee->vmem, thee->pmgp->narr, sizeof(double),
00596         (void *)&(thee->alcf));
00597     Vmem_free(thee->vmem, thee->pmgp->narr, sizeof(double),
00598         (void *)&(thee->a2cf));
00599     Vmem_free(thee->vmem, thee->pmgp->narr, sizeof(double),
00600         (void *)&(thee->a3cf));
00601     Vmem_free(thee->vmem, thee->pmgp->narr, sizeof(double),
00602         (void *)&(thee->ccf));
00603     Vmem_free(thee->vmem, thee->pmgp->narr, sizeof(double),
00604         (void *)&(thee->fcf));
00605     Vmem_free(thee->vmem, thee->pmgp->narr, sizeof(double),
00606         (void *)&(thee->tcf));
00607     Vmem_free(thee->vmem, thee->pmgp->narr, sizeof(double),
00608         (void *)&(thee->u));
00609     Vmem_free(thee->vmem, 5*(thee->pmgp->nx), sizeof(double),
00610         (void *)&(thee->xf));
00611     Vmem_free(thee->vmem, 5*(thee->pmgp->ny), sizeof(double),
00612         (void *)&(thee->yf));
00613     Vmem_free(thee->vmem, 5*(thee->pmgp->nz), sizeof(double),
00614         (void *)&(thee->zf));
00615     Vmem_free(thee->vmem, 10*(thee->pmgp->ny)*(thee->pmgp->nz), sizeof(double),
00616         (void *)&(thee->gxcf));
00617     Vmem_free(thee->vmem, 10*(thee->pmgp->nx)*(thee->pmgp->nz), sizeof(double),
00618         (void *)&(thee->gycf));
00619     Vmem_free(thee->vmem, 10*(thee->pmgp->nx)*(thee->pmgp->ny), sizeof(double),
00620         (void *)&(thee->gzcf));
00621     Vmem_free(thee->vmem, (thee->pmgp->nx)*(thee->pmgp->ny)*(thee->pmgp->nz),
00622         sizeof(double), (void *)&(thee->pvec));
00623
00624     Vmem_dtor(&(thee->vmem));
00625 }
00626
00627 VPUBLIC void Vpmg_setPart(Vpmg *thee, double lowerCorner[3],
00628     double upperCorner[3], int bflags[6]) {
00629
00630     Valist *alist;
00631     Vatom *atom;
00632     int i, j, k, nx, ny, nz;
00633     double xmin, ymin, zmin, x, y, z, hx, hy, hzed, xok, yok, zok;
00634     double x0,x1,y0,y1,z0,z1;
00635
00636     nx = thee->pmgp->nx;
00637     ny = thee->pmgp->ny;
00638     nz = thee->pmgp->nz;
00639     hx = thee->pmgp->hx;
00640     hy = thee->pmgp->hy;
00641     hzed = thee->pmgp->hzed;

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```

00642     xmin = thee->pmgp->xcent - 0.5*hx*(nx-1);
00643     ymin = thee->pmgp->ycent - 0.5*hy*(ny-1);
00644     zmin = thee->pmgp->zcent - 0.5*hzed*(nz-1);
00645
00646     xok = 0;
00647     yok = 0;
00648     zok = 0;
00649
00650     /* We need have called Vpmg_fillco first */
00651
00652     alist = thee->pbe->alist;
00653
00654     Vnm_print(0, "Vpmg_setPart: lower corner = (%g, %g, %g)\n",
00655               lowerCorner[0], lowerCorner[1], lowerCorner[2]);
00656     Vnm_print(0, "Vpmg_setPart: upper corner = (%g, %g, %g)\n",
00657               upperCorner[0], upperCorner[1], upperCorner[2]);
00658     Vnm_print(0, "Vpmg_setPart: actual minima = (%g, %g, %g)\n",
00659               xmin, ymin, zmin);
00660     Vnm_print(0, "Vpmg_setPart: actual maxima = (%g, %g, %g)\n",
00661               xmin+hx*(nx-1), ymin+hy*(ny-1), zmin+hzed*(nz-1));
00662     Vnm_print(0, "Vpmg_setPart: bflag[FRONT] = %d\n",
00663               bflags[VAPBS_FRONT]);
00664     Vnm_print(0, "Vpmg_setPart: bflag[BACK] = %d\n",
00665               bflags[VAPBS_BACK]);
00666     Vnm_print(0, "Vpmg_setPart: bflag[LEFT] = %d\n",
00667               bflags[VAPBS_LEFT]);
00668     Vnm_print(0, "Vpmg_setPart: bflag[RIGHT] = %d\n",
00669               bflags[VAPBS_RIGHT]);
00670     Vnm_print(0, "Vpmg_setPart: bflag[UP] = %d\n",
00671               bflags[VAPBS_UP]);
00672     Vnm_print(0, "Vpmg_setPart: bflag[DOWN] = %d\n",
00673               bflags[VAPBS_DOWN]);
00674
00675     /* Identify atoms as inside, outside, or on the border
00676        If on the border, use the bflags to determine if there
00677        is an adjacent processor - if so, this atom should be equally
00678        shared. */
00679
00680     for (i=0; i<Valist_getNumberAtoms(alist); i++) {
00681         atom = Valist_getAtom(alist, i);
00682
00683         if ((atom->position[0] < upperCorner[0]) &&
00684             (atom->position[0] > lowerCorner[0])) xok = 1;
00685         else {
00686             if ((VABS(atom->position[0] - lowerCorner[0]) < VPMGSMALL) &&
00687                 (bflags[VAPBS_LEFT] == 0)) xok = 1;
00688             else if ((VABS(atom->position[0] - lowerCorner[0]) < VPMGSMALL) &&
00689                     (bflags[VAPBS_LEFT] == 1)) xok = 0.5;
00690             else if ((VABS(atom->position[0] - upperCorner[0]) < VPMGSMALL) &&
00691                     (bflags[VAPBS_RIGHT] == 0)) xok = 1;
00692             else if ((VABS(atom->position[0] - upperCorner[0]) < VPMGSMALL) &&
00693                     (bflags[VAPBS_RIGHT] == 1)) xok = 0.5;
00694             else xok = 0;
00695         }
00696         if ((atom->position[1] < upperCorner[1]) &&
00697             (atom->position[1] > lowerCorner[1])) yok = 1;
00698         else {
00699             if ((VABS(atom->position[1] - lowerCorner[1]) < VPMGSMALL) &&
00700                 (bflags[VAPBS_BACK] == 0)) yok = 1;
00701             else if ((VABS(atom->position[1] - lowerCorner[1]) < VPMGSMALL) &&
00702                     (bflags[VAPBS_BACK] == 1)) yok = 0.5;
00703             else if ((VABS(atom->position[1] - upperCorner[1]) < VPMGSMALL) &&
00704                     (bflags[VAPBS_FRONT] == 0)) yok = 1;
00705             else if ((VABS(atom->position[1] - upperCorner[1]) < VPMGSMALL) &&
00706                     (bflags[VAPBS_FRONT] == 1)) yok = 0.5;
00707             else yok = 0;
00708         }
00709         if ((atom->position[2] < upperCorner[2]) &&
00710             (atom->position[2] > lowerCorner[2])) zok = 1;
00711         else {
00712             if ((VABS(atom->position[2] - lowerCorner[2]) < VPMGSMALL) &&
00713                 (bflags[VAPBS_DOWN] == 0)) zok = 1;
00714             else if ((VABS(atom->position[2] - lowerCorner[2]) < VPMGSMALL) &&
00715                     (bflags[VAPBS_DOWN] == 1)) zok = 0.5;
00716             else if ((VABS(atom->position[2] - upperCorner[2]) < VPMGSMALL) &&
00717                     (bflags[VAPBS_UP] == 0)) zok = 1;
00718             else if ((VABS(atom->position[2] - upperCorner[2]) < VPMGSMALL) &&
00719                     (bflags[VAPBS_UP] == 1)) zok = 0.5;
00720             else zok = 0;
00721         }
00722     }

```

```

00723     atom->partID = xok*yok*zok;
00724     /*
00725     Vnm_print(1, "DEBUG (%s, %d):  atom->position[0] - upperCorner[0] = %g\n",
00726               __FILE__, __LINE__, atom->position[0] - upperCorner[0]);
00727     Vnm_print(1, "DEBUG (%s, %d):  atom->position[0] - lowerCorner[0] = %g\n",
00728               __FILE__, __LINE__, atom->position[0] - lowerCorner[0]);
00729     Vnm_print(1, "DEBUG (%s, %d):  atom->position[1] - upperCorner[1] = %g\n",
00730               __FILE__, __LINE__, atom->position[1] - upperCorner[1]);
00731     Vnm_print(1, "DEBUG (%s, %d):  atom->position[1] - lowerCorner[1] = %g\n",
00732               __FILE__, __LINE__, atom->position[1] - lowerCorner[1]);
00733     Vnm_print(1, "DEBUG (%s, %d):  atom->position[2] - upperCorner[2] = %g\n",
00734               __FILE__, __LINE__, atom->position[2] - upperCorner[2]);
00735     Vnm_print(1, "DEBUG (%s, %d):  atom->position[2] - lowerCorner[0] = %g\n",
00736               __FILE__, __LINE__, atom->position[2] - lowerCorner[2]);
00737     Vnm_print(1, "DEBUG (%s, %d):  xok = %g, yok = %g, zok = %g\n",
00738               __FILE__, __LINE__, xok, yok, zok);
00739     */
00740
00741 }
00742
00743 /* Load up pvec -
00744 For all points within h{axis}/2 of a border - use a gradient
00745 to determine the pvec weight.
00746 Points on the boundary depend on the presence of an adjacent
00747 processor. */
00748
00749 for (i=0; i<(nx*ny*nz); i++) three->pvec[i] = 0.0;
00750
00751 for (i=0; i<nx; i++) {
00752     xok = 0.0;
00753     x = i*hx + xmin;
00754     if ( (x < (upperCorner[0]-hx/2)) &&
00755          (x > (lowerCorner[0]+hx/2))
00756         ) xok = 1.0;
00757     else if ( (VABS(x - lowerCorner[0]) < VPMGSMALL) &&
00758              (bflags[VAPBS_LEFT] == 0) ) xok = 1.0;
00759     else if ( (VABS(x - lowerCorner[0]) < VPMGSMALL) &&
00760              (bflags[VAPBS_LEFT] == 1) ) xok = 0.5;
00761     else if ( (VABS(x - upperCorner[0]) < VPMGSMALL) &&
00762              (bflags[VAPBS_RIGHT] == 0) ) xok = 1.0;
00763     else if ( (VABS(x - upperCorner[0]) < VPMGSMALL) &&
00764              (bflags[VAPBS_RIGHT] == 1) ) xok = 0.5;
00765     else if ((x > (upperCorner[0] + hx/2)) || (x < (lowerCorner[0] - hx/2))) xok = 0.0;
00766     else if ((x < (upperCorner[0] + hx/2)) || (x > (lowerCorner[0] - hx/2))) {
00767         x0 = VMAX2(x - hx/2, lowerCorner[0]);
00768         x1 = VMIN2(x + hx/2, upperCorner[0]);
00769         xok = VABS(x1-x0)/hx;
00770
00771         if (xok < 0.0) {
00772             if (VABS(xok) < VPMGSMALL) xok = 0.0;
00773             else {
00774                 Vnm_print(2, "Vpmg_setPart:  fell off x-interval (%1.12E)!\n",
00775                           xok);
00776                 VASSERT(0);
00777             }
00778         }
00779         if (xok > 1.0) {
00780             if (VABS(xok - 1.0) < VPMGSMALL) xok = 1.0;
00781             else {
00782                 Vnm_print(2, "Vpmg_setPart:  fell off x-interval (%1.12E)!\n",
00783                           xok);
00784                 VASSERT(0);
00785             }
00786         }
00787     }
00788 } else xok = 0.0;
00789
00790 for (j=0; j<ny; j++) {
00791     yok = 0.0;
00792     y = j*hy + ymin;
00793     if ((y < (upperCorner[1]-hy/2)) && (y > (lowerCorner[1]+hy/2))) yok = 1.0;
00794     else if ((VABS(y - lowerCorner[1]) < VPMGSMALL) &&
00795              (bflags[VAPBS_BACK] == 0) ) yok = 1.0;
00796     else if ((VABS(y - lowerCorner[1]) < VPMGSMALL) &&
00797              (bflags[VAPBS_BACK] == 1) ) yok = 0.5;
00798     else if ((VABS(y - upperCorner[1]) < VPMGSMALL) &&
00799              (bflags[VAPBS_FRONT] == 0) ) yok = 1.0;
00800     else if ((VABS(y - upperCorner[1]) < VPMGSMALL) &&
00801              (bflags[VAPBS_FRONT] == 1) ) yok = 0.5;
00802     else if ((y > (upperCorner[1] + hy/2)) || (y < (lowerCorner[1] - hy/2))) yok=0.0;
00803     else if ((y < (upperCorner[1] + hy/2)) || (y > (lowerCorner[1] - hy/2))) {

```

```

00804         y0 = VMAX2(y - hy/2, lowerCorner[1]);
00805         y1 = VMIN2(y + hy/2, upperCorner[1]);
00806         yok = VABS(y1-y0)/hy;
00807
00808         if (yok < 0.0) {
00809             if (VABS(yok) < VPMGSMALL) yok = 0.0;
00810             else {
00811                 Vnm_print(2, "Vpmg_setPart: fell off y-interval (%1.12E)!\n",
00812                     yok);
00813                 VASSERT(0);
00814             }
00815         }
00816         if (yok > 1.0) {
00817             if (VABS(yok - 1.0) < VPMGSMALL) yok = 1.0;
00818             else {
00819                 Vnm_print(2, "Vpmg_setPart: fell off y-interval (%1.12E)!\n",
00820                     yok);
00821                 VASSERT(0);
00822             }
00823         }
00824     }
00825     else yok=0.0;
00826
00827     for (k=0; k<nz; k++) {
00828         zok = 0.0;
00829         z = k*hzed + zmin;
00830         if ((z < (upperCorner[2]-hzed/2)) && (z > (lowerCorner[2]+hzed/2))) zok = 1.0;
00831         else if ((VABS(z - lowerCorner[2]) < VPMGSMALL) &&
00832             (bflags[VAPBS_DOWN] == 0)) zok = 1.0;
00833         else if ((VABS(z - lowerCorner[2]) < VPMGSMALL) &&
00834             (bflags[VAPBS_DOWN] == 1)) zok = 0.5;
00835         else if ((VABS(z - upperCorner[2]) < VPMGSMALL) &&
00836             (bflags[VAPBS_UP] == 0)) zok = 1.0;
00837         else if ((VABS(z - upperCorner[2]) < VPMGSMALL) &&
00838             (bflags[VAPBS_UP] == 1)) zok = 0.5;
00839         else if ((z > (upperCorner[2] + hzed/2)) || (z < (lowerCorner[2] - hzed/2))) zok=0.0;
00840         else if ((z < (upperCorner[2] + hzed/2)) || (z > (lowerCorner[2] - hzed/2))) {
00841             z0 = VMAX2(z - hzed/2, lowerCorner[2]);
00842             z1 = VMIN2(z + hzed/2, upperCorner[2]);
00843             zok = VABS(z1-z0)/hzed;
00844
00845             if (zok < 0.0) {
00846                 if (VABS(zok) < VPMGSMALL) zok = 0.0;
00847                 else {
00848                     Vnm_print(2, "Vpmg_setPart: fell off z-interval (%1.12E)!\n",
00849                         zok);
00850                     VASSERT(0);
00851                 }
00852             }
00853             if (zok > 1.0) {
00854                 if (VABS(zok - 1.0) < VPMGSMALL) zok = 1.0;
00855                 else {
00856                     Vnm_print(2, "Vpmg_setPart: fell off z-interval (%1.12E)!\n",
00857                         zok);
00858                     VASSERT(0);
00859                 }
00860             }
00861         }
00862         else zok = 0.0;
00863
00864         if (VABS(xok*yok*zok) < VPMGSMALL) thee->pvec[IJK(i,j,k)] = 0.0;
00865         else thee->pvec[IJK(i,j,k)] = xok*yok*zok;
00866     }
00867 }
00868 }
00869 }
00870 }
00871
00872 VPUBLIC void Vpmg_unsetPart(Vpmg *thee) {
00873
00874     int i, nx, ny, nz;
00875     Vatom *atom;
00876     Valist *alist;
00877
00878     VASSERT(thee != VNULL);
00879
00880     nx = thee->pmgp->nx;
00881     ny = thee->pmgp->ny;
00882     nz = thee->pmgp->nz;
00883     alist = thee->pbe->alist;
00884

```



```

00885     for (i=0; i<(nx*ny*nz); i++) thee->pvec[i] = 1;
00886     for (i=0; i<Valist_getNumberAtoms(alist); i++) {
00887         atom = Valist_getAtom(alist, i);
00888         atom->partID = 1;
00889     }
00890 }
00891
00892 VPUBLIC int Vpmg_fillArray(Vpmg *thee, double *vec, Vdata_Type type,
00893     double parm, Vhal_PBEType pbetype, PBEparm *pbeparm) {
00894     Vacc *acc = VNULL;
00895     Vpbe *pbe = VNULL;
00896     Vgrid *grid = VNULL;
00897     Vatom *atoms = VNULL;
00898     Valist *alist = VNULL;
00899     double position[3], hx, hy, hzed, xmin, ymin, zmin;
00900     double grad[3], eps, epsp, epss, zmagic, u;
00901     int i, j, k, l, nx, ny, nz, ichop;
00902
00903     pbe = thee->pbe;
00904     acc = Vpbe_getVacc(pbe);
00905     nx = thee->pmgp->nx;
00906     ny = thee->pmgp->ny;
00907     nz = thee->pmgp->nz;
00908     hx = thee->pmgp->hx;
00909     hy = thee->pmgp->hy;
00910     hzed = thee->pmgp->hzed;
00911     xmin = thee->pmgp->xmin;
00912     ymin = thee->pmgp->ymin;
00913     zmin = thee->pmgp->zmin;
00914     epsp = Vpbe_getSoluteDiel(pbe);
00915     epss = Vpbe_getSolventDiel(pbe);
00916     zmagic = Vpbe_getZmagic(pbe);
00917
00918     if (!(thee->filled)) {
00919         Vnm_print(2, "Vpmg_fillArray: need to call Vpmg_fillco first!\n");
00920         return 0;
00921     }
00922 }
00923
00924 switch (type) {
00925     case VDT_CHARGE:
00926         for (i=0; i<nx*ny*nz; i++) vec[i] = thee->charge[i]/zmagic;
00927         break;
00928     case VDT_DIELX:
00929         for (i=0; i<nx*ny*nz; i++) vec[i] = thee->epsx[i];
00930         break;
00931     case VDT_DIELY:
00932         for (i=0; i<nx*ny*nz; i++) vec[i] = thee->epsy[i];
00933         break;
00934     case VDT_DIELZ:
00935         for (i=0; i<nx*ny*nz; i++) vec[i] = thee->epsz[i];
00936         break;
00937     case VDT_KAPPA:
00938         for (i=0; i<nx*ny*nz; i++) vec[i] = thee->kappa[i];
00939         break;
00940     case VDT_POT:
00941         for (i=0; i<nx*ny*nz; i++) vec[i] = thee->u[i];
00942         break;
00943     case VDT_ATOMPOT:
00944         alist = thee->pbe->alist;
00945         atoms = alist[pbeparm->molid-1].atoms;
00946         grid = Vgrid_ctor(nx, ny, nz, hx, hy,
00947             hzed, xmin, ymin, zmin, thee->u);
00948         for (i=0; i<alist[pbeparm->molid-1].number; i++) {
00949             position[0] = atoms[i].position[0];
00950             position[1] = atoms[i].position[1];
00951             position[2] = atoms[i].position[2];
00952         }
00953 }

```

```

00966         Vgrid_value(grid, position, &vec[i]);
00967     }
00968     Vgrid_dtor(&grid);
00969     break;
00970
00971 case VDT_SMOL:
00972     for (k=0; k<nz; k++) {
00973         for (j=0; j<ny; j++) {
00974             for (i=0; i<nx; i++) {
00975
00976                 position[0] = i*hx + xmin;
00977                 position[1] = j*hy + ymin;
00978                 position[2] = k*hzed + zmin;
00979
00980                 vec[IJK(i,j,k)] = (Vacc_molAcc(acc,position,parm));
00981             }
00982         }
00983     }
00984     break;
00985
00986 case VDT_SSPL:
00987     for (k=0; k<nz; k++) {
00988         for (j=0; j<ny; j++) {
00989             for (i=0; i<nx; i++) {
00990
00991                 position[0] = i*hx + xmin;
00992                 position[1] = j*hy + ymin;
00993                 position[2] = k*hzed + zmin;
00994
00995                 vec[IJK(i,j,k)] = Vacc_splineAcc(acc,position,parm,0);
00996             }
00997         }
00998     }
00999     break;
01000
01001 case VDT_VDW:
01002     for (k=0; k<nz; k++) {
01003         for (j=0; j<ny; j++) {
01004             for (i=0; i<nx; i++) {
01005
01006                 position[0] = i*hx + xmin;
01007                 position[1] = j*hy + ymin;
01008                 position[2] = k*hzed + zmin;
01009
01010                 vec[IJK(i,j,k)] = Vacc_vdwAcc(acc,position);
01011             }
01012         }
01013     }
01014     break;
01015
01016 case VDT_IVDW:
01017     for (k=0; k<nz; k++) {
01018         for (j=0; j<ny; j++) {
01019             for (i=0; i<nx; i++) {
01020
01021                 position[0] = i*hx + xmin;
01022                 position[1] = j*hy + ymin;
01023                 position[2] = k*hzed + zmin;
01024
01025                 vec[IJK(i,j,k)] = Vacc_ivdwAcc(acc,position,parm);
01026             }
01027         }
01028     }
01029     break;
01030
01031 case VDT_LAP:
01032     grid = Vgrid_ctor(nx, ny, nz, hx, hy, hzed, xmin, ymin, zmin,
01033         thee->u);
01034     for (k=0; k<nz; k++) {
01035         for (j=0; j<ny; j++) {
01036             for (i=0; i<nx; i++) {
01037
01038                 if ((k==0) || (k==(nz-1)) ||
01039                     (j==0) || (j==(ny-1)) ||
01040                     (i==0) || (i==(nx-1))) {
01041

```

```

01047         vec[IJK(i,j,k)] = 0;
01048     } else {
01049         position[0] = i*hx + xmin;
01050         position[1] = j*hy + ymin;
01051         position[2] = k*hzed + zmin;
01052         VASSERT(Vgrid_curvature(grid,position, 1,
01053             &(vec[IJK(i,j,k)])));
01054     }
01055 }
01056 }
01057 }
01058 }
01059 Vgrid_dtor(&grid);
01060 break;
01061
01062 case VDT_EDENS:
01063     grid = Vgrid_ctor(nx, ny, nz, hx, hy, hzed, xmin, ymin, zmin,
01064         thee->u);
01065     for (k=0; k<nz; k++) {
01066         for (j=0; j<ny; j++) {
01067             for (i=0; i<nx; i++) {
01068                 position[0] = i*hx + xmin;
01069                 position[1] = j*hy + ymin;
01070                 position[2] = k*hzed + zmin;
01071                 VASSERT(Vgrid_gradient(grid, position, grad));
01072                 eps = epsp + (epss-epsp)*Vacc_molAcc(acc, position,
01073                     pbe->solventRadius);
01074                 vec[IJK(i,j,k)] = 0.0;
01075                 for (l=0; l<3; l++)
01076                     vec[IJK(i,j,k)] += eps*VSQR(grad[l]);
01077             }
01078         }
01079     }
01080 }
01081 Vgrid_dtor(&grid);
01082 break;
01083
01084 case VDT_NDENS:
01085     for (k=0; k<nz; k++) {
01086         for (j=0; j<ny; j++) {
01087             for (i=0; i<nx; i++) {
01088                 position[0] = i*hx + xmin;
01089                 position[1] = j*hy + ymin;
01090                 position[2] = k*hzed + zmin;
01091                 vec[IJK(i,j,k)] = 0.0;
01092                 u = thee->u[IJK(i,j,k)];
01093                 if ( VABS(Vacc_ivdwAcc(acc,
01094                     position, pbe->maxIonRadius) - 1.0) < VSMALL) {
01095                     for (l=0; l<pbe->numIon; l++) {
01096                         double q = pbe->ionQ[l];
01097                         if (pbe->pbetype == PBE_NPBE || pbe->pbetype == PBE_SMPBE /* SMPBE Added */) {
01098                             vec[IJK(i,j,k)] += pbe->ionConc[l]*Vcap_exp(-q*u, &ichop);
01099                         } else if (pbe->pbetype == PBE_LPBE){
01100                             vec[IJK(i,j,k)] += pbe->ionConc[l]*(1 - q*u + 0.5*q*q*u*u);
01101                         }
01102                     }
01103                 }
01104             }
01105         }
01106     }
01107 }
01108 }
01109 break;
01110
01111 case VDT_QDENS:
01112     for (k=0; k<nz; k++) {
01113         for (j=0; j<ny; j++) {
01114             for (i=0; i<nx; i++) {
01115                 position[0] = i*hx + xmin;
01116                 position[1] = j*hy + ymin;
01117                 position[2] = k*hzed + zmin;
01118                 vec[IJK(i,j,k)] = 0.0;
01119                 u = thee->u[IJK(i,j,k)];
01120                 if ( VABS(Vacc_ivdwAcc(acc,
01121                     position, pbe->maxIonRadius) - 1.0) < VSMALL) {
01122                     for (l=0; l<pbe->numIon; l++) {
01123                         double q = pbe->ionQ[l];
01124                         if (pbe->pbetype == PBE_NPBE || pbe->pbetype == PBE_SMPBE /* SMPBE Added */) {
01125                             vec[IJK(i,j,k)] += pbe->ionConc[l]*q*Vcap_exp(-q*u, &ichop);
01126                         }
01127                     }
01128                 }
01129             }
01130         }
01131     }
01132 }
01133 break;

```

```

01128         } else if (pbetype == PBE_LPBE) {
01129             vec[IJK(i,j,k)] += pbe->ionConc[1]*q*(1 - q*u + 0.5*q*q*u*u);
01130         }
01131     }
01132 }
01133 }}}
01134 break;
01135
01136 default:
01137     Vnm_print(2, "main: Bogus data type (%d)!\n", type);
01138     return 0;
01139 break;
01140
01141 }
01142
01143 return 1;
01144
01145 }
01146 }
01147
01148 VPRIVATE double Vpmg_polarizEnergy(Vpmg *thee,
01149                                     int extFlag
01150                                     ) {
01151
01152     int i,
01153         j,
01154         k,
01155         ijk,
01156         nx,
01157         ny,
01158         nz,
01159         iatom;
01160     double xmin,
01161            ymin,
01162            zmin,
01163            //x, // gcc: not used
01164            //y,
01165            //z,
01166            hx,
01167            hy,
01168            hzed,
01169            epsp,
01170            lap,
01171            pt[3],
01172            T,
01173            pre,
01174            polq,
01175            dist2,
01176            dist,
01177            energy,
01178            q,
01179            *charge,
01180            *pos,
01181            eps_w;
01182     Vgrid *potgrid;
01183     Vpbe *pbe;
01184     Valist *alist;
01185     Vatom *atom;
01186
01187     xmin = thee->pmgp->xmin;
01188     ymin = thee->pmgp->ymin;
01189     zmin = thee->pmgp->zmin;
01190     hx = thee->pmgp->hx;
01191     hy = thee->pmgp->hy;
01192     hzed = thee->pmgp->hzed;
01193     nx = thee->pmgp->nx;
01194     ny = thee->pmgp->ny;
01195     nz = thee->pmgp->nz;
01196     pbe = thee->pbe;
01197     epsp = Vpbe_getSoluteDiel(pbe);
01198     eps_w = Vpbe_getSolventDiel(pbe);
01199     alist = pbe->alist;
01200     charge = thee->charge;
01201
01202     /* Calculate the prefactor for Coulombic calculations */
01203     T = Vpbe_getTemperature(pbe);
01204     pre = (Vunit_ec*Vunit_ec)/(4*VPI*Vunit_eps0*eps_w*Vunit_kb*T);
01205     pre = pre*(1.0e10);
01206
01207     /* Set up Vgrid object with solution */
01208     potgrid = Vgrid_ctor(nx, ny, nz, hx, hy, hzed, xmin, ymin, zmin, thee->u);

```

```

01209
01210     /* Calculate polarization charge */
01211     energy = 0.0;
01212     for (i=1; i<(nx-1); i++) {
01213         pt[0] = xmin + hx*i;
01214         for (j=1; j<(ny-1); j++) {
01215             pt[1] = ymin + hy*j;
01216             for (k=1; k<(nz-1); k++) {
01217                 pt[2] = zmin + hzed*k;
01218
01219                 /* Calculate polarization charge */
01220                 VASSERT(Vgrid_curvature(potgrid, pt, 1, &lap));
01221                 ijk = IJK(i,j,k);
01222                 polq = charge[ijk] + epsp*lap*3.0;
01223
01224                 /* Calculate interaction energy with atoms */
01225                 if (VABS(polq) > VSMALL) {
01226                     for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
01227                         atom = Valist_getAtom(alist, iatom);
01228                         q = Vatom_getCharge(atom);
01229                         pos = Vatom_getPosition(atom);
01230                         dist2 = VSQR(pos[0]-pt[0]) + VSQR(pos[1]-pt[1]) \
01231                             + VSQR(pos[2]-pt[2]);
01232                         dist = VSQRT(dist2);
01233
01234                         if (dist < VSMALL) {
01235                             Vnm_print(2, "Vpmg_polarizEnergy: atom on grid point; ignoring!\n");
01236                         } else {
01237                             energy = energy + polq*q/dist;
01238                         }
01239                     }
01240                 }
01241             }
01242         }
01243     }
01244
01245     return pre*energy;
01246 }
01247
01248 VPUBLIC double Vpmg_energy(Vpmg *thee,
01249     int extFlag
01250 ) {
01251
01252     double totEnergy = 0.0,
01253         dielEnergy = 0.0,
01254         qmEnergy = 0.0,
01255         qfEnergy = 0.0;
01256
01257     VASSERT(thee != VNULL);
01258
01259     if ((thee->pmgp->nonlin) && (Vpbe_getBulkIonicStrength(thee->pbe) > 0.)) {
01260         Vnm_print(0, "Vpmg_energy: calculating full PBE energy\n");
01261         qmEnergy = Vpmg_qmEnergy(thee, extFlag);
01262         Vnm_print(0, "Vpmg_energy: qmEnergy = %1.12E kT\n", qmEnergy);
01263         qfEnergy = Vpmg_qfEnergy(thee, extFlag);
01264         Vnm_print(0, "Vpmg_energy: qfEnergy = %1.12E kT\n", qfEnergy);
01265         dielEnergy = Vpmg_dielEnergy(thee, extFlag);
01266         Vnm_print(0, "Vpmg_energy: dielEnergy = %1.12E kT\n", dielEnergy);
01267         totEnergy = qfEnergy - dielEnergy - qmEnergy;
01268     } else {
01269         Vnm_print(0, "Vpmg_energy: calculating only q-phi energy\n");
01270         qfEnergy = Vpmg_qfEnergy(thee, extFlag);
01271         Vnm_print(0, "Vpmg_energy: qfEnergy = %1.12E kT\n", qfEnergy);
01272         totEnergy = 0.5*qfEnergy;
01273     }
01274
01275     return totEnergy;
01276 }
01277 }
01278
01279 VPUBLIC double Vpmg_dielEnergy(Vpmg *thee,
01280     int extFlag
01281 ) {
01282
01283     double hx,
01284         hy,
01285         hzed,
01286         energy,
01287         nrgx,
01288         nrgy,
01289         nrgz,

```

```

01290         pvecx,
01291         pvecy,
01292         pvecz;
01293     int i,
01294         j,
01295         k,
01296         nx,
01297         ny,
01298         nz;
01299
01300     VASSERT(thee != VNULL);
01301
01302     /* Get the mesh information */
01303     nx = thee->pmgp->nx;
01304     ny = thee->pmgp->ny;
01305     nz = thee->pmgp->nz;
01306     hx = thee->pmgp->hx;
01307     hy = thee->pmgp->hy;
01308     hzed = thee->pmgp->hzed;
01309
01310     energy = 0.0;
01311
01312     if (!thee->filled) {
01313         Vnm_print(2, "Vpmg_dielEnergy: Need to call Vpmg_fillco!\n");
01314         VASSERT(0);
01315     }
01316
01317     for (k=0; k<(nz-1); k++) {
01318         for (j=0; j<(ny-1); j++) {
01319             for (i=0; i<(nx-1); i++) {
01320                 pvecx = 0.5*(thee->pvec[IJK(i, j, k)]+thee->pvec[IJK(i+1, j, k)]);
01321                 pvecy = 0.5*(thee->pvec[IJK(i, j, k)]+thee->pvec[IJK(i, j+1, k)]);
01322                 pvecz = 0.5*(thee->pvec[IJK(i, j, k)]+thee->pvec[IJK(i, j, k+1)]);
01323                 nrgx = thee->epsx[IJK(i, j, k)]*pvecx
01324                     * VSQR((thee->u[IJK(i, j, k)]-thee->u[IJK(i+1, j, k)]) / hx);
01325                 nrgy = thee->epsy[IJK(i, j, k)]*pvecy
01326                     * VSQR((thee->u[IJK(i, j, k)]-thee->u[IJK(i, j+1, k)]) / hy);
01327                 nrgz = thee->epsz[IJK(i, j, k)]*pvecz
01328                     * VSQR((thee->u[IJK(i, j, k)]-thee->u[IJK(i, j, k+1)]) / hzed);
01329                 energy += (nrgx + nrgy + nrgz);
01330             }
01331         }
01332     }
01333
01334     energy = 0.5*energy*hx*hy*hzed;
01335     energy = energy/Vpbe_getZmagic(thee->pbe);
01336
01337     if (extFlag == 1) energy += (thee->extDiEnergy);
01338
01339     return energy;
01340 }
01341
01342 VPUBLIC double Vpmg_dielGradNorm(Vpmg *thee) {
01343
01344     double hx, hy, hzed, energy, nrgx, nrgy, nrgz, pvecx, pvecy, pvecz;
01345     int i, j, k, nx, ny, nz;
01346
01347     VASSERT(thee != VNULL);
01348
01349     /* Get the mesh information */
01350     nx = thee->pmgp->nx;
01351     ny = thee->pmgp->ny;
01352     nz = thee->pmgp->nz;
01353     hx = thee->pmgp->hx;
01354     hy = thee->pmgp->hy;
01355     hzed = thee->pmgp->hzed;
01356
01357     energy = 0.0;
01358
01359     if (!thee->filled) {
01360         Vnm_print(2, "Vpmg_dielGradNorm: Need to call Vpmg_fillco!\n");
01361         VASSERT(0);
01362     }
01363
01364     for (k=1; k<nz; k++) {
01365         for (j=1; j<ny; j++) {
01366             for (i=1; i<nx; i++) {
01367                 pvecx = 0.5*(thee->pvec[IJK(i, j, k)]+thee->pvec[IJK(i-1, j, k)]);
01368                 pvecy = 0.5*(thee->pvec[IJK(i, j, k)]+thee->pvec[IJK(i, j-1, k)]);
01369                 pvecz = 0.5*(thee->pvec[IJK(i, j, k)]+thee->pvec[IJK(i, j, k-1)]);
01370                 nrgx = pvecx

```

```

01371         * VSQR((thee->epsx[IJK(i,j,k)]-thee->epsx[IJK(i-1,j,k)]) /hx);
01372         nrgy = pvecy
01373         * VSQR((thee->epsy[IJK(i,j,k)]-thee->epsy[IJK(i,j-1,k)]) /hy);
01374         nrgz = pvecz
01375         * VSQR((thee->epsz[IJK(i,j,k)]-thee->epsz[IJK(i,j,k-1)]) /hzed);
01376         energy += VSQRT(nrgx + nrgy + nrgz);
01377     }
01378 }
01379 }
01380
01381 energy = energy*hx*hy*hzed;
01382
01383 return energy;
01384 }
01385
01386 VPUBLIC double Vpmg_qmEnergy(Vpmg *thee,
01387                             int extFlag
01388                             ) {
01389     double energy;
01390
01391     if(thee->pbe->ipkey == IPKEY_SMPBE){
01392         energy = Vpmg_qmEnergySMPBE(thee,extFlag);
01393     }else{
01394         energy = Vpmg_qmEnergyNONLIN(thee,extFlag);
01395     }
01396 }
01397
01398 return energy;
01399 }
01400
01401 VPRIVATE double Vpmg_qmEnergyNONLIN(Vpmg *thee,
01402                                     int extFlag
01403                                     ) {
01404     double hx,
01405            hy,
01406            hzed,
01407            energy,
01408            ionConc[MAXION],
01409            ionRadii[MAXION],
01410            ionQ[MAXION],
01411            zkappa2,
01412            ionstr,
01413            zks2;
01414     int i, /* Loop variable */
01415         j,
01416         nx,
01417         ny,
01418         nz,
01419         nion,
01420         ichop,
01421         nchop,
01422         len; /* Stores number of iterations for loops to avoid multiple recalculations */
01423
01424     VASSERT(thee != VNULL);
01425
01426     /* Get the mesh information */
01427     nx = thee->pmgp->nx;
01428     ny = thee->pmgp->ny;
01429     nz = thee->pmgp->nz;
01430     hx = thee->pmgp->hx;
01431     hy = thee->pmgp->hy;
01432     hzed = thee->pmgp->hzed;
01433     zkappa2 = Vpbe_getZkappa2(thee->pbe);
01434     ionstr = Vpbe_getBulkIonicStrength(thee->pbe);
01435
01436     /* Bail if we're at zero ionic strength */
01437     if (zkappa2 < VSMALL) {
01438         #ifndef VAPBSQUIET
01439             Vnm_print(0, "Vpmg_qmEnergy: Zero energy for zero ionic strength!\n");
01440         #endif
01441         return 0.0;
01442     }
01443     zks2 = 0.5*zkappa2/ionstr;
01444
01445     if (!thee->filled) {
01446         Vnm_print(2, "Vpmg_qmEnergy: Need to call Vpmg_fillco()!\n");
01447         VASSERT(0);
01448     }
01449 }

```

```

01452
01453     energy = 0.0;
01454     nchop = 0;
01455     Vpbe_getIons(thee->pbe, &nion, ionConc, ionRadii, ionQ);
01456     if (thee->pmgp->nonlin) {
01457         Vnm_print(0, "Vpmg_qmEnergy: Calculating nonlinear energy\n");
01458         for (i=0, len=nx*ny*nz; i<len; i++) {
01459             if (thee->pvec[i]*thee->kappa[i] > VSMALL) {
01460                 for (j=0; j<nion; j++) {
01461                     energy += (thee->pvec[i]*thee->kappa[i]*zks2
01462                             * ionConc[j]
01463                             * (Vcap_exp(-ionQ[j]*thee->u[i], &ichop)-1.0));
01464                     nchop += ichop;
01465                 }
01466             }
01467         }
01468         if (nchop > 0) {
01469             Vnm_print(2, "Vpmg_qmEnergy: Chopped EXP %d times!\n", nchop);
01470             Vnm_print(2, "\nERROR! Detected large potential values in energy evaluation! \nERROR! This
calculation failed -- please report to the APBS developers!\n\n");
01471             VASSERT(0);
01472         }
01473     } else {
01474         /* Zkappa2 OK here b/c LPBE approx */
01475         Vnm_print(0, "Vpmg_qmEnergy: Calculating linear energy\n");
01476         for (i=0, len=nx*ny*nz; i<len; i++) {
01477             if (thee->pvec[i]*thee->kappa[i] > VSMALL)
01478                 energy += (thee->pvec[i]*zkappa2*thee->kappa[i]*VSQR(thee->u[i]));
01479         }
01480         energy = 0.5*energy;
01481     }
01482     energy = energy*hx*hy*hzed;
01483     energy = energy/Vpbe_getZmagic(thee->pbe);
01484
01485     if (extFlag == 1) energy += thee->extQmEnergy;
01486
01487     return energy;
01488 }
01489
01490 VPUBLIC double Vpmg_qmEnergySMPBE(Vpmg *thee,
01491                                 int extFlag
01492                                 ) {
01493
01494     double hx,
01495            hy,
01496            hzed,
01497            energy,
01498            ionConc[MAXION],
01499            ionRadii[MAXION],
01500            ionQ[MAXION],
01501            zkappa2,
01502            ionstr,
01503            zks2;
01504     int i,
01505         //j, // gcc: not used
01506         nx,
01507         ny,
01508         nz,
01509         nion,
01510         //ichop, // gcc: not used
01511         nchop,
01512         len; /* Loop variable */
01513
01514     /* SMPB Modification (vchu, 09/21/06)*/
01515     /* variable declarations for SMPB energy terms */
01516     double a,
01517            k,
01518            z1,
01519            z2,
01520            z3,
01521            cb1,
01522            cb2,
01523            cb3,
01524            a1,
01525            a2,
01526            a3,
01527            c1,
01528            c2,
01529            c3,
01530            currEnergy,
01531            fracOccA,

```



```

01532         fracOccB,
01533         fracOccC,
01534         phi,
01535         gpark,
01536         denom;
01537         // Na; /**< @todo remove if no conflicts are caused - This constant is already defined in
vpde.h. no need to redefine. */
01538         int ichop1,
01539         ichop2,
01540         ichop3;
01541
01542         VASSERT(thee != VNULL);
01543
01544         /* Get the mesh information */
01545         nx = thee->pmgp->nx;
01546         ny = thee->pmgp->ny;
01547         nz = thee->pmgp->nz;
01548         hx = thee->pmgp->hx;
01549         hy = thee->pmgp->hy;
01550         hzed = thee->pmgp->hzed;
01551         zkappa2 = Vpbe_getZkappa2(thee->pbe);
01552         ionstr = Vpbe_getBulkIonicStrength(thee->pbe);
01553
01554         /* Bail if we're at zero ionic strength */
01555         if (zkappa2 < VSMALL) {
01556
01557 #ifndef VAPBSQUIET
01558             Vnm_print(0, "Vpmg_qmEnergySMPBE: Zero energy for zero ionic strength!\n");
01559 #endif
01560
01561             return 0.0;
01562         }
01563         zks2 = 0.5*zkappa2/ionstr;
01564
01565         if (!thee->filled) {
01566             Vnm_print(2, "Vpmg_qmEnergySMPBE: Need to call Vpmg_fillco()!\n");
01567             VASSERT(0);
01568         }
01569
01570         energy = 0.0;
01571         nchop = 0;
01572         Vpbe_getIons(thee->pbe, &nion, ionConc, ionRadii, ionQ);
01573
01574         /* SMPB Modification (vchu, 09/21/06) */
01575         /* Extensive modification to the first part of the if statement
01576            where that handles the thee->pmgp->nonlin part. Basically, I've
01577            deleted all of the original code and written my own code that computes
01578            the electrostatic free energy in the SMPB framework. Definitely really hacky
01579            at this stage of the game, but gets the job done. The second part of the
01580            if statement (the part that handles linear poisson-boltzmann) has been deleted
01581            because there will be no linearized SMPB energy.. */
01582
01583         z1 = ionQ[0];
01584         z2 = ionQ[1];
01585         z3 = ionQ[2];
01586         cb1 = ionConc[0];
01587         cb2 = ionConc[1];
01588         cb3 = ionConc[2];
01589         a = thee->pbe->smvolume;
01590         k = thee->pbe->smsize;
01591
01592         // This constant is defined in vpde.h Do not need to redefine
01593         //Na = 6.022045000e-04; /* Converts from Molar to N/A^3 */
01594
01595         fracOccA = Na*cb1*VCUB(a);
01596         fracOccB = Na*cb2*VCUB(a);
01597         fracOccC = Na*cb3*VCUB(a);
01598
01599         phi = (fracOccA/k) + fracOccB + fracOccC;
01600
01601         if (thee->pmgp->nonlin) {
01602             Vnm_print(0, "Vpmg_qmEnergySMPBE: Calculating nonlinear energy using SMPB functional!\n");
01603             for (i=0, len=nx*ny*nz; i<len; i++) {
01604                 if ((k-1) > VSMALL) && (thee->pvec[i]*thee->kappa[i] > VSMALL)) {
01605
01606                     a1 = Vcap_exp(-1.0*z1*thee->u[i], &ichop1);
01607                     a2 = Vcap_exp(-1.0*z2*thee->u[i], &ichop2);
01608                     a3 = Vcap_exp(-1.0*z3*thee->u[i], &ichop3);
01609
01610                     nchop += ichop1 + ichop2 + ichop3;
01611
01612

```

```

01613         gpark = (1 - phi + (fracOccA/k)*a1);
01614         denom = VPOW(gpark, k) + VPOW(1-fracOccB-fracOccC, k-1)*(fracOccB*a2+fracOccC*a3);
01615
01616         if (cb1 > VSMALL) {
01617             c1 = Na*cb1*VPOW(gpark, k-1)*a1/denom;
01618             if(c1 != c1) c1 = 0.;
01619         } else c1 = 0.;
01620
01621         if (cb2 > VSMALL) {
01622             c2 = Na*cb2*VPOW(1-fracOccB-fracOccC,k-1)*a2/denom;
01623             if(c2 != c2) c2 = 0.;
01624         } else c2 = 0.;
01625
01626         if (cb3 > VSMALL) {
01627             c3 = Na*cb3*VPOW(1-fracOccB-fracOccC,k-1)*a3/denom;
01628             if(c3 != c3) c3 = 0.;
01629         } else c3 = 0.;
01630
01631         currEnergy = k*VLOG((1-(c1*VCUB(a)/k)-c2*VCUB(a)-c3*VCUB(a))/(1-phi))
01632             -(k-1)*VLOG((1-c2*VCUB(a)-c3*VCUB(a))/(1-phi+(fracOccA/k)));
01633
01634         energy += thee->pvec[i]*thee->kappa[i]*currEnergy;
01635
01636     } else if (thee->pvec[i]*thee->kappa[i] > VSMALL){
01637
01638         a1 = Vcap_exp(-1.0*z1*thee->u[i], &ichop1);
01639         a2 = Vcap_exp(-1.0*z2*thee->u[i], &ichop2);
01640         a3 = Vcap_exp(-1.0*z3*thee->u[i], &ichop3);
01641
01642         nchop += ichop1 + ichop2 + ichop3;
01643
01644         gpark = (1 - phi + (fracOccA)*a1);
01645         denom = gpark + (fracOccB*a2+fracOccC*a3);
01646
01647         if (cb1 > VSMALL) {
01648             c1 = Na*cb1*a1/denom;
01649             if(c1 != c1) c1 = 0.;
01650         } else c1 = 0.;
01651
01652         if (cb2 > VSMALL) {
01653             c2 = Na*cb2*a2/denom;
01654             if(c2 != c2) c2 = 0.;
01655         } else c2 = 0.;
01656
01657         if (cb3 > VSMALL) {
01658             c3 = Na*cb3*a3/denom;
01659             if(c3 != c3) c3 = 0.;
01660         } else c3 = 0.;
01661
01662         currEnergy = VLOG((1-c1*VCUB(a)-c2*VCUB(a)-c3*VCUB(a))/(1-fracOccA-fracOccB-fracOccC));
01663
01664         energy += thee->pvec[i]*thee->kappa[i]*currEnergy;
01665     }
01666 }
01667
01668 energy = -energy/VCUB(a);
01669
01670 if (nchop > 0) Vnm_print(2, "Vpmg_qmEnergySMPBE: Chopped EXP %d times!\n",
01671     nchop);
01672
01673 } else {
01674     /* Zkappa2 OK here b/c LPBE approx */
01675     Vnm_print(0, "Vpmg_qmEnergySMPBE: ERROR: NO LINEAR ENERGY!! Returning 0!\n");
01676
01677     energy = 0.0;
01678
01679 }
01680 energy = energy*hx*hy*hzed;
01681
01682 if (extFlag == 1) energy += thee->extQmEnergy;
01683
01684 return energy;
01685 }
01686
01687 VPUBLIC double Vpmg_qfEnergy(Vpmg *thee,
01688     int extFlag
01689 ) {
01690
01691     double energy = 0.0;
01692
01693     VASSERT(thee != VNULL);

```

```

01694
01695     if ((thee->useChargeMap) || (thee->chargeMeth == VCM_BSPL2)) {
01696         energy = Vpmg_qfEnergyVolume(thee, extFlag);
01697     } else {
01698         energy = Vpmg_qfEnergyPoint(thee, extFlag);
01699     }
01700
01701     return energy;
01702 }
01703
01704 VPRIVATE double Vpmg_qfEnergyPoint(Vpmg *thee,
01705                                     int extFlag
01706                                     ) {
01707
01708     int iatom, nx, ny, nz, ihi, ilo, jhi, jlo, khi, klo;
01709     double xmax, ymax, zmax, xmin, ymin, zmin, hx, hy, hzed, ifloat, jfloat;
01710     double charge, kfloat, dx, dy, dz, energy, uval, *position;
01711     double *u;
01712     double *pvec;
01713     Valist *alist;
01714     Vatom *atom;
01715     Vpbe *pbe;
01716
01717     pbe = thee->pbe;
01718     alist = pbe->alist;
01719     VASSERT(alist != VNULL);
01720
01721     /* Get the mesh information */
01722     nx = thee->pmgp->nx;
01723     ny = thee->pmgp->ny;
01724     nz = thee->pmgp->nz;
01725     hx = thee->pmgp->hx;
01726     hy = thee->pmgp->hy;
01727     hzed = thee->pmgp->hzed;
01728     xmax = thee->pmgp->xmax;
01729     ymax = thee->pmgp->ymax;
01730     zmax = thee->pmgp->zmax;
01731     xmin = thee->pmgp->xmin;
01732     ymin = thee->pmgp->ymin;
01733     zmin = thee->pmgp->zmin;
01734
01735     u = thee->u;
01736     pvec = thee->pvec;
01737
01738     energy = 0.0;
01739
01740     for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
01741
01742         /* Get atomic information */
01743         atom = Valist_getAtom(alist, iatom);
01744
01745         position = Vatom_getPosition(atom);
01746         charge = Vatom_getCharge(atom);
01747
01748         /* Figure out which vertices we're next to */
01749         ifloat = (position[0] - xmin)/hx;
01750         jfloat = (position[1] - ymin)/hy;
01751         kfloat = (position[2] - zmin)/hzed;
01752         ihi = (int)ceil(ifloat);
01753         ilo = (int)floor(ifloat);
01754         jhi = (int)ceil(jfloat);
01755         jlo = (int)floor(jfloat);
01756         khi = (int)ceil(kfloat);
01757         klo = (int)floor(kfloat);
01758
01759         if (atom->partID > 0) {
01760
01761             if ((ihi<nx) && (jhi<ny) && (khi<nz) &&
01762                 (ilo>=0) && (jlo>=0) && (klo>=0)) {
01763
01764                 /* Now get trilinear interpolation constants */
01765                 dx = ifloat - (double)(ilo);
01766                 dy = jfloat - (double)(jlo);
01767                 dz = kfloat - (double)(klo);
01768                 uval =
01769                     dx*dy*dz*u[IJK(ihi, jhi, khi)]
01770                     + dx*(1.0-dy)*dz*u[IJK(ihi, jlo, khi)]
01771                     + dx*dy*(1.0-dz)*u[IJK(ihi, jhi, klo)]
01772                     + dx*(1.0-dy)*(1.0-dz)*u[IJK(ihi, jlo, klo)]
01773                     + (1.0-dx)*dy*dz*u[IJK(ilo, jhi, khi)]
01774                     + (1.0-dx)*(1.0-dy)*dz*u[IJK(ilo, jlo, khi)]

```

```

01775         + (1.0-dx)*dy*(1.0-dz)*u[IJK(ilo,jhi,klo)]
01776         + (1.0-dx)*(1.0-dy)*(1.0-dz)*u[IJK(ilo,jlo,klo)];
01777         energy += (uval*charge*atom->partID);
01778     } else if (three->pmg->bcfl != BCFL_FOCUS) {
01779         Vnm_print(2, "Vpmg_qfEnergy: Atom #%d at (%4.3f, %4.3f, \
01780 %4.3f) is off the mesh (ignoring)!\n",
01781         iatom, position[0], position[1], position[2]);
01782     }
01783 }
01784 }
01785
01786 if (extFlag) energy += three->extQfEnergy;
01787
01788 return energy;
01789 }
01790
01791 VPUBLIC double Vpmg_qfAtomEnergy(Vpmg *three, Vatom *atom) {
01792
01793     int nx, ny, nz, ihi, ilo, jhi, jlo, khi, klo;
01794     double xmax, xmin, ymax, ymin, zmax, zmin, hx, hy, hzed, ifloat, jfloat;
01795     double charge, kfloat, dx, dy, dz, energy, uval, *position;
01796     double *u;
01797
01798     /* Get the mesh information */
01799     nx = three->pmg->nx;
01800     ny = three->pmg->ny;
01801     nz = three->pmg->nz;
01802     hx = three->pmg->hx;
01803     hy = three->pmg->hy;
01804     hzed = three->pmg->hzed;
01805     xmax = three->xf[nx-1];
01806     ymax = three->yf[ny-1];
01807     zmax = three->zf[nz-1];
01808     xmin = three->xf[0];
01809     ymin = three->yf[0];
01810     zmin = three->zf[0];
01811
01812     u = three->u;
01813
01814     energy = 0.0;
01815
01816
01817     position = Vatom_getPosition(atom);
01818     charge = Vatom_getCharge(atom);
01819
01820     /* Figure out which vertices we're next to */
01821     ifloat = (position[0] - xmin)/hx;
01822     jfloat = (position[1] - ymin)/hy;
01823     kfloat = (position[2] - zmin)/hzed;
01824     ihi = (int)ceil(ifloat);
01825     ilo = (int)floor(ifloat);
01826     jhi = (int)ceil(jfloat);
01827     jlo = (int)floor(jfloat);
01828     khi = (int)ceil(kfloat);
01829     klo = (int)floor(kfloat);
01830
01831     if (atom->partID > 0) {
01832
01833         if ((ihi<nx) && (jhi<ny) && (khi<nz) &&
01834             (ilo>=0) && (jlo>=0) && (klo>=0)) {
01835
01836             /* Now get trilinear interpolation constants */
01837             dx = ifloat - (double)(ilo);
01838             dy = jfloat - (double)(jlo);
01839             dz = kfloat - (double)(klo);
01840             uval =
01841                 dx*dy*dz*u[IJK(ihi,jhi,khi)]
01842                 + dx*(1.0-dy)*dz*u[IJK(ihi,jlo,khi)]
01843                 + dx*dy*(1.0-dz)*u[IJK(ihi,jhi,klo)]
01844                 + dx*(1.0-dy)*(1.0-dz)*u[IJK(ihi,jlo,klo)]
01845                 + (1.0-dx)*dy*dz*u[IJK(ilo,jhi,khi)]
01846                 + (1.0-dx)*(1.0-dy)*dz*u[IJK(ilo,jlo,khi)]
01847                 + (1.0-dx)*dy*(1.0-dz)*u[IJK(ilo,jhi,klo)]
01848                 + (1.0-dx)*(1.0-dy)*(1.0-dz)*u[IJK(ilo,jlo,klo)];
01849             energy += (uval*charge*atom->partID);
01850         } else if (three->pmg->bcfl != BCFL_FOCUS) {
01851             Vnm_print(2, "Vpmg_qfAtomEnergy: Atom at (%4.3f, %4.3f, \
01852 %4.3f) is off the mesh (ignoring)!\n",
01853             position[0], position[1], position[2]);
01854         }
01855     }

```

```

01856     }
01857
01858     return energy;
01859 }
01860
01861 VPRIVATE double Vpmg_qfEnergyVolume(Vpmg *thee, int extFlag) {
01862     double hx, hy, hzed, energy;
01863     int i, nx, ny, nz;
01864
01865     VASSERT(thee != VNULL);
01866
01867     /* Get the mesh information */
01868     nx = thee->pmgp->nx;
01869     ny = thee->pmgp->ny;
01870     nz = thee->pmgp->nz;
01871     hx = thee->pmgp->hx;
01872     hy = thee->pmgp->hy;
01873     hzed = thee->pmgp->hzed;
01874
01875     if (!thee->filled) {
01876         Vnm_print(2, "Vpmg_qfEnergyVolume: need to call Vpmg_fillco!\n");
01877         VASSERT(0);
01878     }
01879
01880     energy = 0.0;
01881     Vnm_print(0, "Vpmg_qfEnergyVolume: Calculating energy\n");
01882     for (i=0; i<(nx*ny*nz); i++) {
01883         energy += (thee->pvec[i]*thee->u[i]*thee->charge[i]);
01884     }
01885     energy = energy*hx*hy*hzed/Vpbe_getZmagic(thee->pbe);
01886
01887     if (extFlag == 1) energy += thee->extQfEnergy;
01888
01889     return energy;
01890 }
01891
01892 VPRIVATE void Vpmg_splineSelect(int srfm, Vacc *acc, double *gpos, double win,
01893                                 double infrad, Vatom *atom, double *force){
01894
01895     switch (srfm) {
01896         case VSM_SPLINE :
01897             Vacc_splineAccGradAtomNorm(acc, gpos, win, infrad, atom, force);
01898             break;
01899         case VSM_SPLINE3:
01900             Vacc_splineAccGradAtomNorm3(acc, gpos, win, infrad, atom, force);
01901             break;
01902         case VSM_SPLINE4 :
01903             Vacc_splineAccGradAtomNorm4(acc, gpos, win, infrad, atom, force);
01904             break;
01905         default:
01906             Vnm_print(2, "Vpmg_dbnbForce: Unknown surface method.\n");
01907             return;
01908     }
01909
01910     return;
01911 }
01912
01913 VPRIVATE void focusFillBound(Vpmg *thee,
01914                              Vpmg *pmgOLD
01915                              ) {
01916
01917     Vpbe *pbe;
01918     double hxOLD,
01919            hyOLD,
01920            hzOLD,
01921            xminOLD,
01922            yminOLD,
01923            zminOLD,
01924            xmaxOLD,
01925            ymaxOLD,
01926            zmaxOLD,
01927            hxNEW,
01928            hyNEW,
01929            hzNEW,
01930            xminNEW,
01931            yminNEW,
01932            zminNEW,
01933            xmaxNEW,
01934            ymaxNEW,
01935            zmaxNEW,

```

```

01937         x,
01938         y,
01939         z,
01940         dx,
01941         dy,
01942         dz,
01943         ifloat,
01944         jfloat,
01945         kfloat,
01946         uval,
01947         eps_w,
01948         T,
01949         prel,
01950         xkappa,
01951         size,
01952         *apos,
01953         charge,
01954         //pos[3], // gcc: not used
01955         uvalMin,
01956         uvalMax,
01957         *data;
01958     int nxOLD,
01959         nyOLD,
01960         nzOLD,
01961         nxNEW,
01962         nyNEW,
01963         nzNEW,
01964         i,
01965         j,
01966         k,
01967         ihi,
01968         ilo,
01969         jhi,
01970         jlo,
01971         khi,
01972         klo,
01973         nx,
01974         ny,
01975         nz;
01976
01977     /* Calculate new problem dimensions */
01978     hxNEW = thee->pmgp->hx;
01979     hyNEW = thee->pmgp->hy;
01980     hzNEW = thee->pmgp->hz;
01981     nx = thee->pmgp->nx;
01982     ny = thee->pmgp->ny;
01983     nz = thee->pmgp->nz;
01984     nxNEW = thee->pmgp->nx;
01985     nyNEW = thee->pmgp->ny;
01986     nzNEW = thee->pmgp->nz;
01987     xminNEW = thee->pmgp->xcent - ((double) (nxNEW-1) * hxNEW) / 2.0;
01988     xmaxNEW = thee->pmgp->xcent + ((double) (nxNEW-1) * hxNEW) / 2.0;
01989     yminNEW = thee->pmgp->ycent - ((double) (nyNEW-1) * hyNEW) / 2.0;
01990     ymaxNEW = thee->pmgp->ycent + ((double) (nyNEW-1) * hyNEW) / 2.0;
01991     zminNEW = thee->pmgp->zcent - ((double) (nzNEW-1) * hzNEW) / 2.0;
01992     zmaxNEW = thee->pmgp->zcent + ((double) (nzNEW-1) * hzNEW) / 2.0;
01993
01994     if (pmgOLD != VNULL) {
01995         /* Relevant old problem parameters */
01996         hxOLD = pmgOLD->pmgp->hx;
01997         hyOLD = pmgOLD->pmgp->hy;
01998         hzOLD = pmgOLD->pmgp->hz;
01999         nxOLD = pmgOLD->pmgp->nx;
02000         nyOLD = pmgOLD->pmgp->ny;
02001         nzOLD = pmgOLD->pmgp->nz;
02002         xminOLD = pmgOLD->pmgp->xcent - ((double) (nxOLD-1) * hxOLD) / 2.0;
02003         xmaxOLD = pmgOLD->pmgp->xcent + ((double) (nxOLD-1) * hxOLD) / 2.0;
02004         yminOLD = pmgOLD->pmgp->ycent - ((double) (nyOLD-1) * hyOLD) / 2.0;
02005         ymaxOLD = pmgOLD->pmgp->ycent + ((double) (nyOLD-1) * hyOLD) / 2.0;
02006         zminOLD = pmgOLD->pmgp->zcent - ((double) (nzOLD-1) * hzOLD) / 2.0;
02007         zmaxOLD = pmgOLD->pmgp->zcent + ((double) (nzOLD-1) * hzOLD) / 2.0;
02008
02009         data = pmgOLD->u;
02010     } else {
02011         /* Relevant old problem parameters */
02012         hxOLD = thee->potMap->hx;
02013         hyOLD = thee->potMap->hy;
02014         hzOLD = thee->potMap->hz;
02015         nxOLD = thee->potMap->nx;
02016         nyOLD = thee->potMap->ny;
02017         nzOLD = thee->potMap->nz;

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02018     xminOLD = thee->potMap->xmin;
02019     xmaxOLD = thee->potMap->xmax;
02020     yminOLD = thee->potMap->ymin;
02021     ymaxOLD = thee->potMap->ymax;
02022     zminOLD = thee->potMap->zmin;
02023     zmaxOLD = thee->potMap->zmax;
02024
02025     data = thee->potMap->data;
02026 }
02027 /* BOUNDARY CONDITION SETUP FOR POINTS OFF OLD MESH:
02028  * For each "atom" (only one for bcfl=1), we use the following formula to
02029  * calculate the boundary conditions:
02030  *  $g(x) = \frac{q e_c}{4\pi\epsilon_0\epsilon_w k_b T} \frac{\exp(-\kappa(d-a))}{1+\kappa a}$ 
02031  *  $\frac{1}{d}$ 
02032  * where  $d = ||x - x_0||$  (in m) and  $a$  is the size of the atom (in m).
02033  * We only need to evaluate some of these prefactors once:
02034  *  $prel = \frac{e_c}{4\pi\epsilon_0\epsilon_w k_b T}$ 
02035  * which gives the potential as
02036  *  $g(x) = prel * q/d * \frac{\exp(-\kappa(d-a))}{1+\kappa a}$ 
02037  */
02038
02039 pbe = thee->pbe;
02040 eps_w = Vpbe_getSolventDiel(pbe); /* Dimensionless */
02041 T = Vpbe_getTemperature(pbe); /* K */
02042 prel = (Vunit_ec)/(4*VPI*Vunit_eps0*eps_w*Vunit_kb*T);
02043
02044 /* Finally, if we convert keep xkappa in A^{-1} and scale prel by
02045  * m/A, then we will only need to deal with distances and sizes in
02046  * Angstroms rather than meters. */
02047 xkappa = Vpbe_getXkappa(pbe); /* A^{-1} */
02048 prel = prel*(1.0e10);
02049 size = Vpbe_getSoluteRadius(pbe);
02050 apos = Vpbe_getSoluteCenter(pbe);
02051 charge = Vunit_ec*Vpbe_getSoluteCharge(pbe);
02052
02053 /* Check for rounding error */
02054 if (VABS(xminOLD-xminNEW) < VSMALL) xminNEW = xminOLD;
02055 if (VABS(xmaxOLD-xmaxNEW) < VSMALL) xmaxNEW = xmaxOLD;
02056 if (VABS(yminOLD-yminNEW) < VSMALL) yminNEW = yminOLD;
02057 if (VABS(ymaxOLD-ymaxNEW) < VSMALL) ymaxNEW = ymaxOLD;
02058 if (VABS(zminOLD-zminNEW) < VSMALL) zminNEW = zminOLD;
02059 if (VABS(zmaxOLD-zmaxNEW) < VSMALL) zmaxNEW = zmaxOLD;
02060
02061
02062 /* Sanity check: make sure we're within the old mesh */
02063 Vnm_print(0, "VPMG::focusFillBound -- New mesh mins = %g, %g, %g\n",
02064     xminNEW, yminNEW, zminNEW);
02065 Vnm_print(0, "VPMG::focusFillBound -- New mesh maxs = %g, %g, %g\n",
02066     xmaxNEW, ymaxNEW, zmaxNEW);
02067 Vnm_print(0, "VPMG::focusFillBound -- Old mesh mins = %g, %g, %g\n",
02068     xminOLD, yminOLD, zminOLD);
02069 Vnm_print(0, "VPMG::focusFillBound -- Old mesh maxs = %g, %g, %g\n",
02070     xmaxOLD, ymaxOLD, zmaxOLD);
02071
02072 /* The following is obsolete; we'll substitute analytical boundary
02073  * condition values when the new mesh falls outside the old */
02074 if ((xmaxNEW>xmaxOLD) || (ymaxNEW>ymaxOLD) || (zmaxNEW>zmaxOLD) ||
02075     (xminOLD>xminNEW) || (yminOLD>yminNEW) || (zminOLD>zminNEW)) {
02076
02077     Vnm_print(2, "Vpmg::focusFillBound -- new mesh not contained in old!\n");
02078     Vnm_print(2, "Vpmg::focusFillBound -- old mesh min = (%g, %g, %g)\n",
02079         xminOLD, yminOLD, zminOLD);
02080     Vnm_print(2, "Vpmg::focusFillBound -- old mesh max = (%g, %g, %g)\n",
02081         xmaxOLD, ymaxOLD, zmaxOLD);
02082     Vnm_print(2, "Vpmg::focusFillBound -- new mesh min = (%g, %g, %g)\n",
02083         xminNEW, yminNEW, zminNEW);
02084     Vnm_print(2, "Vpmg::focusFillBound -- new mesh max = (%g, %g, %g)\n",
02085         xmaxNEW, ymaxNEW, zmaxNEW);
02086     fflush(stderr);
02087     VASSERT(0);
02088 }
02089
02090 uvalMin = VPMGSMALL;
02091 uvalMax = -VPMGSMALL;
02092
02093 /* Fill the "i" boundaries (dirichlet) */
02094 for (k=0; k<nzNEW; k++) {
02095     for (j=0; j<nyNEW; j++) {
02096         /* Low X face */
02097         x = xminNEW;
02098         y = yminNEW + j*hyNEW;

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02099      z = zminNEW + k*hzNEW;
02100      if ((x >= (xminOLD-VSMALL)) && (y >= (yminOLD-VSMALL)) && (z >= (zminOLD-VSMALL)) &&
02101          (x <= (xmaxOLD+VSMALL)) && (y <= (ymaxOLD+VSMALL)) && (z <= (zmaxOLD+VSMALL))) {
02102          ifloat = (x - xminOLD)/hxOLD;
02103          jfloat = (y - yminOLD)/hyOLD;
02104          kfloat = (z - zminOLD)/hzOLD;
02105          ihi = (int)ceil(ifloat);
02106          if (ihi > (nxOLD-1)) ihi = nxOLD-1;
02107          ilo = (int)floor(ifloat);
02108          if (ilo < 0) ilo = 0;
02109          jhi = (int)ceil(jfloat);
02110          if (jhi > (nyOLD-1)) jhi = nyOLD-1;
02111          jlo = (int)floor(jfloat);
02112          if (jlo < 0) jlo = 0;
02113          khi = (int)ceil(kfloat);
02114          if (khi > (nzOLD-1)) khi = nzOLD-1;
02115          klo = (int)floor(kfloat);
02116          if (klo < 0) klo = 0;
02117          dx = ifloat - (double)(ilo);
02118          dy = jfloat - (double)(jlo);
02119          dz = kfloat - (double)(klo);
02120          nx = nxOLD; ny = nyOLD; nz = nzOLD;
02121          uval = dx*dy*dz*(data[IJK(ihi,jhi,khi)])
02122                + dx*(1.0-dy)*dz*(data[IJK(ihi,jlo,khi)])
02123                + dx*dy*(1.0-dz)*(data[IJK(ihi,jhi,klo)])
02124                + dx*(1.0-dy)*(1.0-dz)*(data[IJK(ihi,jlo,klo)])
02125                + (1.0-dx)*dy*dz*(data[IJK(ilo,jhi,khi)])
02126                + (1.0-dx)*(1.0-dy)*dz*(data[IJK(ilo,jlo,khi)])
02127                + (1.0-dx)*dy*(1.0-dz)*(data[IJK(ilo,jhi,klo)])
02128                + (1.0-dx)*(1.0-dy)*(1.0-dz)*(data[IJK(ilo,jlo,klo)]);
02129          nx = nxNEW; ny = nyNEW; nz = nzNEW;
02130      } else {
02131          Vnm_print(2, "focusFillBound (%s, %d): Off old mesh at %g, %g \
02132                  %g!\n", __FILE__, __LINE__, x, y, z);
02133          Vnm_print(2, "focusFillBound (%s, %d): old mesh lower corner at \
02134                  %g %g %g.\n", __FILE__, __LINE__, xminOLD, yminOLD, zminOLD);
02135          Vnm_print(2, "focusFillBound (%s, %d): old mesh upper corner at \
02136                  %g %g %g.\n", __FILE__, __LINE__, xmaxOLD, ymaxOLD, zmaxOLD);
02137          VASSERT(0);
02138      }
02139      nx = nxNEW; ny = nyNEW; nz = nzNEW;
02140      thee->gxcf[IJKx(j,k,0)] = uval;
02141      if(uval < uvalMin) uvalMin = uval;
02142      if(uval > uvalMax) uvalMax = uval;
02143
02144      /* High X face */
02145      x = xmaxNEW;
02146      if ((x >= (xminOLD-VSMALL)) && (y >= (yminOLD-VSMALL)) && (z >= (zminOLD-VSMALL)) &&
02147          (x <= (xmaxOLD+VSMALL)) && (y <= (ymaxOLD+VSMALL)) && (z <= (zmaxOLD+VSMALL))) {
02148          ifloat = (x - xminOLD)/hxOLD;
02149          jfloat = (y - yminOLD)/hyOLD;
02150          kfloat = (z - zminOLD)/hzOLD;
02151          ihi = (int)ceil(ifloat);
02152          if (ihi > (nxOLD-1)) ihi = nxOLD-1;
02153          ilo = (int)floor(ifloat);
02154          if (ilo < 0) ilo = 0;
02155          jhi = (int)ceil(jfloat);
02156          if (jhi > (nyOLD-1)) jhi = nyOLD-1;
02157          jlo = (int)floor(jfloat);
02158          if (jlo < 0) jlo = 0;
02159          khi = (int)ceil(kfloat);
02160          if (khi > (nzOLD-1)) khi = nzOLD-1;
02161          klo = (int)floor(kfloat);
02162          if (klo < 0) klo = 0;
02163          dx = ifloat - (double)(ilo);
02164          dy = jfloat - (double)(jlo);
02165          dz = kfloat - (double)(klo);
02166          nx = nxOLD; ny = nyOLD; nz = nzOLD;
02167          uval = dx*dy*dz*(data[IJK(ihi,jhi,khi)])
02168                + dx*(1.0-dy)*dz*(data[IJK(ihi,jlo,khi)])
02169                + dx*dy*(1.0-dz)*(data[IJK(ihi,jhi,klo)])
02170                + dx*(1.0-dy)*(1.0-dz)*(data[IJK(ihi,jlo,klo)])
02171                + (1.0-dx)*dy*dz*(data[IJK(ilo,jhi,khi)])
02172                + (1.0-dx)*(1.0-dy)*dz*(data[IJK(ilo,jlo,khi)])
02173                + (1.0-dx)*dy*(1.0-dz)*(data[IJK(ilo,jhi,klo)])
02174                + (1.0-dx)*(1.0-dy)*(1.0-dz)*(data[IJK(ilo,jlo,klo)]);
02175          nx = nxNEW; ny = nyNEW; nz = nzNEW;
02176      } else {
02177          Vnm_print(2, "focusFillBound (%s, %d): Off old mesh at %g, %g \
02178                  %g!\n", __FILE__, __LINE__, x, y, z);
02179          Vnm_print(2, "focusFillBound (%s, %d): old mesh lower corner at \

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02180         %g %g %g.\n", __FILE__, __LINE__, xminOLD, yminOLD, zminOLD);
02181     Vnm_print(2, "focusFillBound (%s, %d): old mesh upper corner at \
02182         %g %g %g.\n", __FILE__, __LINE__, xmaxOLD, ymaxOLD, zmaxOLD);
02183     VASSERT(0);
02184 }
02185 nx = nxNEW; ny = nyNEW; nz = nzNEW;
02186 thee->gxcf[IJKx(j,k,1)] = uval;
02187 if(uval < uvalMin) uvalMin = uval;
02188 if(uval > uvalMax) uvalMax = uval;
02189
02190 /* Zero Neumann conditions */
02191 nx = nxNEW; ny = nyNEW; nz = nzNEW;
02192 thee->gxcf[IJKx(j,k,2)] = 0.0;
02193 nx = nxNEW; ny = nyNEW; nz = nzNEW;
02194 thee->gxcf[IJKx(j,k,3)] = 0.0;
02195 }
02196 }
02197
02198 /* Fill the "j" boundaries (dirichlet) */
02199 for (k=0; k<nzNEW; k++) {
02200     for (i=0; i<nxNEW; i++) {
02201         /* Low Y face */
02202         x = xminNEW + i*hxNEW;
02203         y = yminNEW;
02204         z = zminNEW + k*hzNEW;
02205         if ((x >= (xminOLD-VSMALL)) && (y >= (yminOLD-VSMALL)) && (z >= (zminOLD-VSMALL)) &&
02206             (x <= (xmaxOLD+VSMALL)) && (y <= (ymaxOLD+VSMALL)) && (z <= (zmaxOLD+VSMALL))) {
02207             ifloat = (x - xminOLD)/hxOLD;
02208             jfloat = (y - yminOLD)/hyOLD;
02209             kfloat = (z - zminOLD)/hzOLD;
02210             ihi = (int)ceil(ifloat);
02211             if (ihi > (nxOLD-1)) ihi = nxOLD-1;
02212             ilo = (int)floor(ifloat);
02213             if (ilo < 0) ilo = 0;
02214             jhi = (int)ceil(jfloat);
02215             if (jhi > (nyOLD-1)) jhi = nyOLD-1;
02216             jlo = (int)floor(jfloat);
02217             if (jlo < 0) jlo = 0;
02218             khi = (int)ceil(kfloat);
02219             if (khi > (nzOLD-1)) khi = nzOLD-1;
02220             klo = (int)floor(kfloat);
02221             if (klo < 0) klo = 0;
02222             dx = ifloat - (double)(ilo);
02223             dy = jfloat - (double)(jlo);
02224             dz = kfloat - (double)(klo);
02225             nx = nxOLD; ny = nyOLD; nz = nzOLD;
02226             uval = dx*dy*dz*(data[IJK(ihi,jhi,khi)])
02227                 + dx*(1.0-dy)*dz*(data[IJK(ihi,jlo,khi)])
02228                 + dx*dy*(1.0-dz)*(data[IJK(ihi,jhi,klo)])
02229                 + dx*(1.0-dy)*(1.0-dz)*(data[IJK(ihi,jlo,klo)])
02230                 + (1.0-dx)*dy*dz*(data[IJK(ilo,jhi,khi)])
02231                 + (1.0-dx)*(1.0-dy)*dz*(data[IJK(ilo,jlo,khi)])
02232                 + (1.0-dx)*dy*(1.0-dz)*(data[IJK(ilo,jhi,klo)])
02233                 + (1.0-dx)*(1.0-dy)*(1.0-dz)*(data[IJK(ilo,jlo,klo)]);
02234             nx = nxNEW; ny = nyNEW; nz = nzNEW;
02235         } else {
02236             Vnm_print(2, "focusFillBound (%s, %d): Off old mesh at %g, %g \
02237                 %g!\n", __FILE__, __LINE__, x, y, z);
02238             Vnm_print(2, "focusFillBound (%s, %d): old mesh lower corner at \
02239                 %g %g %g.\n", __FILE__, __LINE__, xminOLD, yminOLD, zminOLD);
02240             Vnm_print(2, "focusFillBound (%s, %d): old mesh upper corner at \
02241                 %g %g %g.\n", __FILE__, __LINE__, xmaxOLD, ymaxOLD, zmaxOLD);
02242             VASSERT(0);
02243         }
02244         nx = nxNEW; ny = nyNEW; nz = nzNEW;
02245         thee->gycf[IJKy(i,k,0)] = uval;
02246         if(uval < uvalMin) uvalMin = uval;
02247         if(uval > uvalMax) uvalMax = uval;
02248
02249         /* High Y face */
02250         y = ymaxNEW;
02251         if ((x >= (xminOLD-VSMALL)) && (y >= (yminOLD-VSMALL)) && (z >= (zminOLD-VSMALL)) &&
02252             (x <= (xmaxOLD+VSMALL)) && (y <= (ymaxOLD+VSMALL)) && (z <= (zmaxOLD+VSMALL))) {
02253             ifloat = (x - xminOLD)/hxOLD;
02254             jfloat = (y - yminOLD)/hyOLD;
02255             kfloat = (z - zminOLD)/hzOLD;
02256             ihi = (int)ceil(ifloat);
02257             if (ihi > (nxOLD-1)) ihi = nxOLD-1;
02258             ilo = (int)floor(ifloat);
02259             if (ilo < 0) ilo = 0;
02260             jhi = (int)ceil(jfloat);

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02261         if (jhi > (nyOLD-1)) jhi = nyOLD-1;
02262         jlo = (int)floor(jfloat);
02263         if (jlo < 0) jlo = 0;
02264         khi = (int)ceil(kfloat);
02265         if (khi > (nzOLD-1)) khi = nzOLD-1;
02266         klo = (int)floor(kfloat);
02267         if (klo < 0) klo = 0;
02268         dx = ifloat - (double)(ilo);
02269         dy = jfloat - (double)(jlo);
02270         dz = kfloat - (double)(klo);
02271         nx = nxOLD; ny = nyOLD; nz = nzOLD;
02272         uval = dx*dy*dz*(data[IJK(ihi,jhi,khi)])
02273         + dx*(1.0-dy)*dz*(data[IJK(ihi,jlo,khi)])
02274         + dx*dy*(1.0-dz)*(data[IJK(ihi,jhi,klo)])
02275         + dx*(1.0-dy)*(1.0-dz)*(data[IJK(ihi,jlo,klo)])
02276         + (1.0-dx)*dy*dz*(data[IJK(ilo,jhi,khi)])
02277         + (1.0-dx)*(1.0-dy)*dz*(data[IJK(ilo,jlo,khi)])
02278         + (1.0-dx)*dy*(1.0-dz)*(data[IJK(ilo,jhi,klo)])
02279         + (1.0-dx)*(1.0-dy)*(1.0-dz)*(data[IJK(ilo,jlo,klo)]);
02280         nx = nxNEW; ny = nyNEW; nz = nzNEW;
02281     } else {
02282         Vnm_print(2, "focusFillBound (%s, %d): Off old mesh at %g, %g \
02283             %g!\n", __FILE__, __LINE__, x, y, z);
02284         Vnm_print(2, "focusFillBound (%s, %d): old mesh lower corner at \
02285             %g %g %g.\n", __FILE__, __LINE__, xminOLD, yminOLD, zminOLD);
02286         Vnm_print(2, "focusFillBound (%s, %d): old mesh upper corner at \
02287             %g %g %g.\n", __FILE__, __LINE__, xmaxOLD, ymaxOLD, zmaxOLD);
02288         VASSERT(0);
02289     }
02290     nx = nxNEW; ny = nyNEW; nz = nzNEW;
02291     thee->gycf[IJKy(i,k,1)] = uval;
02292     if(uval < uvalMin) uvalMin = uval;
02293     if(uval > uvalMax) uvalMax = uval;
02294
02295     /* Zero Neumann conditions */
02296     nx = nxNEW; ny = nyNEW; nz = nzNEW;
02297     thee->gycf[IJKy(i,k,2)] = 0.0;
02298     nx = nxNEW; ny = nyNEW; nz = nzNEW;
02299     thee->gycf[IJKy(i,k,3)] = 0.0;
02300 }
02301 }
02302
02303 /* Fill the "k" boundaries (dirichlet) */
02304 for (j=0; j<nyNEW; j++) {
02305     for (i=0; i<nxNEW; i++) {
02306         /* Low Z face */
02307         x = xminNEW + i*hxNEW;
02308         y = yminNEW + j*hyNEW;
02309         z = zminNEW;
02310         if ((x >= (xminOLD-VSMALL)) && (y >= (yminOLD-VSMALL)) && (z >= (zminOLD-VSMALL)) &&
02311             (x <= (xmaxOLD+VSMALL)) && (y <= (ymaxOLD+VSMALL)) && (z <= (zmaxOLD+VSMALL))) {
02312             ifloat = (x - xminOLD)/hxOLD;
02313             jfloat = (y - yminOLD)/hyOLD;
02314             kfloat = (z - zminOLD)/hzOLD;
02315             ihi = (int)ceil(ifloat);
02316             if (ihi > (nxOLD-1)) ihi = nxOLD-1;
02317             ilo = (int)floor(ifloat);
02318             if (ilo < 0) ilo = 0;
02319             jhi = (int)ceil(jfloat);
02320             if (jhi > (nyOLD-1)) jhi = nyOLD-1;
02321             jlo = (int)floor(jfloat);
02322             if (jlo < 0) jlo = 0;
02323             khi = (int)ceil(kfloat);
02324             if (khi > (nzOLD-1)) khi = nzOLD-1;
02325             klo = (int)floor(kfloat);
02326             if (klo < 0) klo = 0;
02327             dx = ifloat - (double)(ilo);
02328             dy = jfloat - (double)(jlo);
02329             dz = kfloat - (double)(klo);
02330             nx = nxOLD; ny = nyOLD; nz = nzOLD;
02331             uval = dx*dy*dz*(data[IJK(ihi,jhi,khi)])
02332             + dx*(1.0-dy)*dz*(data[IJK(ihi,jlo,khi)])
02333             + dx*dy*(1.0-dz)*(data[IJK(ihi,jhi,klo)])
02334             + dx*(1.0-dy)*(1.0-dz)*(data[IJK(ihi,jlo,klo)])
02335             + (1.0-dx)*dy*dz*(data[IJK(ilo,jhi,khi)])
02336             + (1.0-dx)*(1.0-dy)*dz*(data[IJK(ilo,jlo,khi)])
02337             + (1.0-dx)*dy*(1.0-dz)*(data[IJK(ilo,jhi,klo)])
02338             + (1.0-dx)*(1.0-dy)*(1.0-dz)*(data[IJK(ilo,jlo,klo)]);
02339             nx = nxNEW; ny = nyNEW; nz = nzNEW;
02340         } else {
02341             Vnm_print(2, "focusFillBound (%s, %d): Off old mesh at %g, %g \

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02342         %g!\n", __FILE__, __LINE__, x, y, z);
02343     Vnm_print(2, "focusFillBound (%s, %d): old mesh lower corner at \
02344     %g %g %g.\n", __FILE__, __LINE__, xminOLD, yminOLD, zminOLD);
02345     Vnm_print(2, "focusFillBound (%s, %d): old mesh upper corner at \
02346     %g %g %g.\n", __FILE__, __LINE__, xmaxOLD, ymaxOLD, zmaxOLD);
02347     VASSERT(0);
02348 }
02349 nx = nxNEW; ny = nyNEW; nz = nzNEW;
02350 thee->gzcf[IJKz(i,j,0)] = uval;
02351 if(uval < uvalMin) uvalMin = uval;
02352 if(uval > uvalMax) uvalMax = uval;
02353
02354 /* High Z face */
02355 z = zmaxNEW;
02356 if ((x >= (xminOLD-VSMALL)) && (y >= (yminOLD-VSMALL)) && (z >= (zminOLD-VSMALL)) &&
02357     (x <= (xmaxOLD+VSMALL)) && (y <= (ymaxOLD+VSMALL)) && (z <= (zmaxOLD+VSMALL))) {
02358     ifloat = (x - xminOLD)/hxOLD;
02359     jfloat = (y - yminOLD)/hyOLD;
02360     kfloat = (z - zminOLD)/hzOLD;
02361     ihi = (int)ceil(ifloat);
02362     if (ihi > (nxOLD-1)) ihi = nxOLD-1;
02363     ilo = (int)floor(ifloat);
02364     if (ilo < 0) ilo = 0;
02365     jhi = (int)ceil(jfloat);
02366     if (jhi > (nyOLD-1)) jhi = nyOLD-1;
02367     jlo = (int)floor(jfloat);
02368     if (jlo < 0) jlo = 0;
02369     khi = (int)ceil(kfloat);
02370     if (khi > (nzOLD-1)) khi = nzOLD-1;
02371     klo = (int)floor(kfloat);
02372     if (klo < 0) klo = 0;
02373     dx = ifloat - (double)(ilo);
02374     dy = jfloat - (double)(jlo);
02375     dz = kfloat - (double)(klo);
02376     nx = nxOLD; ny = nyOLD; nz = nzOLD;
02377     uval = dx*dy*dz*(data[IJK(ihi,jhi,khi)])
02378     + dx*(1.0-dy)*dz*(data[IJK(ihi,jlo,khi)])
02379     + dx*dy*(1.0-dz)*(data[IJK(ihi,jhi,klo)])
02380     + dx*(1.0-dy)*(1.0-dz)*(data[IJK(ihi,jlo,klo)])
02381     + (1.0-dx)*dy*dz*(data[IJK(ilo,jhi,khi)])
02382     + (1.0-dx)*(1.0-dy)*dz*(data[IJK(ilo,jlo,khi)])
02383     + (1.0-dx)*dy*(1.0-dz)*(data[IJK(ilo,jhi,klo)])
02384     + (1.0-dx)*(1.0-dy)*(1.0-dz)*(data[IJK(ilo,jlo,klo)]);
02385     nx = nxNEW; ny = nyNEW; nz = nzNEW;
02386 } else {
02387     Vnm_print(2, "focusFillBound (%s, %d): Off old mesh at %g, %g \
02388     %g!\n", __FILE__, __LINE__, x, y, z);
02389     Vnm_print(2, "focusFillBound (%s, %d): old mesh lower corner at \
02390     %g %g %g.\n", __FILE__, __LINE__, xminOLD, yminOLD, zminOLD);
02391     Vnm_print(2, "focusFillBound (%s, %d): old mesh upper corner at \
02392     %g %g %g.\n", __FILE__, __LINE__, xmaxOLD, ymaxOLD, zmaxOLD);
02393     VASSERT(0);
02394 }
02395 nx = nxNEW; ny = nyNEW; nz = nzNEW;
02396 thee->gzcf[IJKz(i,j,1)] = uval;
02397 if(uval < uvalMin) uvalMin = uval;
02398 if(uval > uvalMax) uvalMax = uval;
02399
02400 /* Zero Neumann conditions */
02401 nx = nxNEW; ny = nyNEW; nz = nzNEW;
02402 thee->gzcf[IJKz(i,j,2)] = 0.0;
02403 nx = nxNEW; ny = nyNEW; nz = nzNEW;
02404 thee->gzcf[IJKz(i,j,3)] = 0.0;
02405 }
02406 }
02407
02408 VWARN_MSG0(
02409     uvalMin >= SINH_MIN && uvalMax <= SINH_MAX,
02410     "Unusually large potential values\n"
02411     " detected on the focusing boundary!\n"
02412     " Convergence not guaranteed for NPBE/NRPBE calculations!"
02413 );
02414 }
02415
02416 VPRIVATE void extEnergy(Vpmg *thee, Vpmg *pmgOLD, PBEparm_calcEnergy extFlag,
02417     double partMin[3], double partMax[3], int bflags[6]) {
02418
02419     Vatom *atom;
02420     double hxNEW, hyNEW, hzNEW;
02421     double lowerCorner[3], upperCorner[3];
02422     int nxNEW, nyNEW, nzNEW;

```

```

02423     int nxOLD, nyOLD, nzOLD;
02424     int i,j,k;
02425     double xmin, xmax, ymin, ymax, zmin, zmax;
02426     double hxOLD, hyOLD, hzOLD;
02427     double xval, yval, zval;
02428     double x,y,z;
02429     int nx, ny, nz;
02430
02431     /* Set the new external energy contribution to zero. Any external
02432      * contributions from higher levels will be included in the appropriate
02433      * energy function call. */
02434     thee->extQmEnergy = 0;
02435     thee->extQfEnergy = 0;
02436     thee->extDiEnergy = 0;
02437
02438     /* New problem dimensions */
02439     hxNEW = thee->pmgp->hx;
02440     hyNEW = thee->pmgp->hy;
02441     hzNEW = thee->pmgp->hz;
02442     nxNEW = thee->pmgp->nx;
02443     nyNEW = thee->pmgp->ny;
02444     nzNEW = thee->pmgp->nz;
02445     lowerCorner[0] = thee->pmgp->xcent - ((double) (nxNEW-1)*hxNEW)/2.0;
02446     upperCorner[0] = thee->pmgp->xcent + ((double) (nxNEW-1)*hxNEW)/2.0;
02447     lowerCorner[1] = thee->pmgp->ycent - ((double) (nyNEW-1)*hyNEW)/2.0;
02448     upperCorner[1] = thee->pmgp->ycent + ((double) (nyNEW-1)*hyNEW)/2.0;
02449     lowerCorner[2] = thee->pmgp->zcent - ((double) (nzNEW-1)*hzNEW)/2.0;
02450     upperCorner[2] = thee->pmgp->zcent + ((double) (nzNEW-1)*hzNEW)/2.0;
02451
02452     Vnm_print(0, "VPMG::extEnergy:  energy flag = %d\n", extFlag);
02453
02454     /* Old problem dimensions */
02455     nxOLD = pmgOLD->pmgp->nx;
02456     nyOLD = pmgOLD->pmgp->ny;
02457     nzOLD = pmgOLD->pmgp->nz;
02458
02459     /* Create a partition based on the new problem dimensions */
02460     /* Vnm_print(1, "DEBUG (%s, %d):  extEnergy calling Vpmg_setPart for old PMG.\n",
02461      * _FILE_, _LINE_); */
02462     Vpmg_setPart(pmgOLD, lowerCorner, upperCorner, bflags);
02463
02464
02465     Vnm_print(0, "VPMG::extEnergy:  Finding extEnergy dimensions...\n");
02466     Vnm_print(0, "VPMG::extEnergy  Disj part lower corner = (%g, %g, %g)\n",
02467       partMin[0], partMin[1], partMin[2]);
02468     Vnm_print(0, "VPMG::extEnergy  Disj part upper corner = (%g, %g, %g)\n",
02469       partMax[0], partMax[1], partMax[2]);
02470
02471     /* Find the old dimensions */
02472
02473     hxOLD = pmgOLD->pmgp->hx;
02474     hyOLD = pmgOLD->pmgp->hy;
02475     hzOLD = pmgOLD->pmgp->hz;
02476     xmin = pmgOLD->pmgp->xcent - 0.5*hxOLD*(nxOLD-1);
02477     ymin = pmgOLD->pmgp->ycent - 0.5*hyOLD*(nyOLD-1);
02478     zmin = pmgOLD->pmgp->zcent - 0.5*hzOLD*(nzOLD-1);
02479     xmax = xmin+hxOLD*(nxOLD-1);
02480     ymax = ymin+hyOLD*(nyOLD-1);
02481     zmax = zmin+hzOLD*(nzOLD-1);
02482
02483     Vnm_print(0, "VPMG::extEnergy  Old lower corner = (%g, %g, %g)\n",
02484       xmin, ymin, zmin);
02485     Vnm_print(0, "VPMG::extEnergy  Old upper corner = (%g, %g, %g)\n",
02486       xmax, ymax, zmax);
02487
02488     /* Flip the partition, but do not include any points that will
02489      * be included by another processor */
02490
02491     nx = nxOLD;
02492     ny = nyOLD;
02493     nz = nzOLD;
02494
02495     for(i=0; i<nx; i++) {
02496         xval = 1;
02497         x = i*hxOLD + xmin;
02498         if (x < partMin[0] && bflags[VAPBS_LEFT] == 1) xval = 0;
02499         else if (x > partMax[0] && bflags[VAPBS_RIGHT] == 1) xval = 0;
02500
02501         for(j=0; j<ny; j++) {
02502             yval = 1;
02503             y = j*hyOLD + ymin;

```

```

02504         if (y < partMin[1] && bflags[VAPBS_BACK] == 1) yval = 0;
02505     else if (y > partMax[1] && bflags[VAPBS_FRONT] == 1) yval = 0;
02506
02507     for(k=0; k<nz; k++) {
02508         zval = 1;
02509         z = k*hzOLD + zmin;
02510         if (z < partMin[2] && bflags[VAPBS_DOWN] == 1) zval = 0;
02511         else if (z > partMax[2] && bflags[VAPBS_UP] == 1) zval = 0;
02512
02513         if (pmgOLD->pvec[IJK(i,j,k)] > VSMALL) pmgOLD->pvec[IJK(i,j,k)] = 1.0;
02514         pmgOLD->pvec[IJK(i,j,k)] = (1 - (pmgOLD->pvec[IJK(i,j,k)])) * (xval*yval*zval);
02515     }
02516 }
02517 }
02518
02519 for (i=0; i<Valist_getNumberAtoms(thee->pbe->alist); i++) {
02520     xval=1;
02521     yval=1;
02522     zval=1;
02523     atom = Valist_getAtom(thee->pbe->alist, i);
02524     x = atom->position[0];
02525     y = atom->position[1];
02526     z = atom->position[2];
02527     if (x < partMin[0] && bflags[VAPBS_LEFT] == 1) xval = 0;
02528     else if (x > partMax[0] && bflags[VAPBS_RIGHT] == 1) xval = 0;
02529     if (y < partMin[1] && bflags[VAPBS_BACK] == 1) yval = 0;
02530     else if (y > partMax[1] && bflags[VAPBS_FRONT] == 1) yval = 0;
02531     if (z < partMin[2] && bflags[VAPBS_DOWN] == 1) zval = 0;
02532     else if (z > partMax[2] && bflags[VAPBS_UP] == 1) zval = 0;
02533     if (atom->partID > VSMALL) atom->partID = 1.0;
02534     atom->partID = (1 - atom->partID) * (xval*yval*zval);
02535 }
02536
02537 /* Now calculate the energy on inverted subset of the domain */
02538 thee->extQmEnergy = Vpmg_qmEnergy(pmgOLD, 1);
02539 Vnm_print(0, "VPMG::extEnergy: extQmEnergy = %g kT\n", thee->extQmEnergy);
02540 thee->extQfEnergy = Vpmg_qfEnergy(pmgOLD, 1);
02541 Vnm_print(0, "VPMG::extEnergy: extQfEnergy = %g kT\n", thee->extQfEnergy);
02542 thee->extDiEnergy = Vpmg_dielEnergy(pmgOLD, 1);
02543 Vnm_print(0, "VPMG::extEnergy: extDiEnergy = %g kT\n", thee->extDiEnergy);
02544 Vpmg_unsetPart(pmgOLD);
02545 }
02546
02547 VPRIVATE double bcfl1sp(double size, double *apos, double charge,
02548                        double xkappa, double prel, double *pos) {
02549
02550     double dist, val;
02551
02552     dist = VSQR(VSQR(pos[0]-apos[0]) + VSQR(pos[1]-apos[1])
02553               + VSQR(pos[2]-apos[2]));
02554     if (xkappa > VSMALL) {
02555         val = prel*(charge/dist)*VEXP(-xkappa*(dist-size))
02556             / (1+xkappa*size);
02557     } else {
02558         val = prel*(charge/dist);
02559     }
02560
02561     return val;
02562 }
02563
02564 VPRIVATE void bcfl1(double size, double *apos, double charge,
02565                   double xkappa, double prel, double *gxcf, double *gycf, double *gzcf,
02566                   double *xf, double *yf, double *zf, int nx, int ny, int nz) {
02567
02568     int i, j, k;
02569     double dist, val;
02570     double gpos[3];
02571
02572     /* the "i" boundaries (dirichlet) */
02573     for (k=0; k<nz; k++) {
02574         gpos[2] = zf[k];
02575         for (j=0; j<ny; j++) {
02576             gpos[1] = yf[j];
02577             gpos[0] = xf[0];
02578             dist = VSQR(VSQR(gpos[0]-apos[0]) + VSQR(gpos[1]-apos[1])
02579                     + VSQR(gpos[2]-apos[2]));
02580             if (xkappa > VSMALL) {
02581                 val = prel*(charge/dist)*VEXP(-xkappa*(dist-size))
02582                     / (1+xkappa*size);
02583             } else {
02584                 val = prel*(charge/dist);

```

```

02585         }
02586         gxcf[IJKx(j,k,0)] += val;
02587         gpos[0] = xf[nx-1];
02588         dist = VSQRT(VSQR(gpos[0]-apos[0]) + VSQR(gpos[1]-apos[1])
02589                     + VSQR(gpos[2]-apos[2]));
02590         if (xkappa > VSMALL) {
02591             val = prel*(charge/dist)*VEXP(-xkappa*(dist-size))
02592                 / (1+xkappa*size);
02593         } else {
02594             val = prel*(charge/dist);
02595         }
02596         gxcf[IJKx(j,k,1)] += val;
02597     }
02598 }
02599
02600 /* the "j" boundaries (dirichlet) */
02601 for (k=0; k<nz; k++) {
02602     gpos[2] = zf[k];
02603     for (i=0; i<nx; i++) {
02604         gpos[0] = xf[i];
02605         gpos[1] = yf[0];
02606         dist = VSQRT(VSQR(gpos[0]-apos[0]) + VSQR(gpos[1]-apos[1])
02607                     + VSQR(gpos[2]-apos[2]));
02608         if (xkappa > VSMALL) {
02609             val = prel*(charge/dist)*VEXP(-xkappa*(dist-size))
02610                 / (1+xkappa*size);
02611         } else {
02612             val = prel*(charge/dist);
02613         }
02614         gycf[IJKy(i,k,0)] += val;
02615         gpos[1] = yf[ny-1];
02616         dist = VSQRT(VSQR(gpos[0]-apos[0]) + VSQR(gpos[1]-apos[1])
02617                     + VSQR(gpos[2]-apos[2]));
02618         if (xkappa > VSMALL) {
02619             val = prel*(charge/dist)*VEXP(-xkappa*(dist-size))
02620                 / (1+xkappa*size);
02621         } else {
02622             val = prel*(charge/dist);
02623         }
02624         gycf[IJKy(i,k,1)] += val;
02625     }
02626 }
02627
02628 /* the "k" boundaries (dirichlet) */
02629 for (j=0; j<ny; j++) {
02630     gpos[1] = yf[j];
02631     for (i=0; i<nx; i++) {
02632         gpos[0] = xf[i];
02633         gpos[2] = zf[0];
02634         dist = VSQRT(VSQR(gpos[0]-apos[0]) + VSQR(gpos[1]-apos[1])
02635                     + VSQR(gpos[2]-apos[2]));
02636         if (xkappa > VSMALL) {
02637             val = prel*(charge/dist)*VEXP(-xkappa*(dist-size))
02638                 / (1+xkappa*size);
02639         } else {
02640             val = prel*(charge/dist);
02641         }
02642         gzcfc[IJKz(i,j,0)] += val;
02643         gpos[2] = zf[nz-1];
02644         dist = VSQRT(VSQR(gpos[0]-apos[0]) + VSQR(gpos[1]-apos[1])
02645                     + VSQR(gpos[2]-apos[2]));
02646         if (xkappa > VSMALL) {
02647             val = prel*(charge/dist)*VEXP(-xkappa*(dist-size))
02648                 / (1+xkappa*size);
02649         } else {
02650             val = prel*(charge/dist);
02651         }
02652         gzcfc[IJKz(i,j,1)] += val;
02653     }
02654 }
02655 }
02656
02657 VPRIVATE void bcfl2(double size, double *apos,
02658                   double charge, double *dipole, double *quad,
02659                   double xkappa, double eps_p, double eps_w, double T,
02660                   double *gxcf, double *gycf, double *gzcfc,
02661                   double *xf, double *yf, double *zf,
02662                   int nx, int ny, int nz) {
02663
02664     int i, j, k;
02665     double val;

```

```

02666     double gpos[3], tensor[3];
02667     double ux, uy, uz, xr, yr, zr;
02668     double qxx, qxy, qxz, qyx, qyy, qyz, qzx, qzy, qzz;
02669     double dist, pre;
02670
02671     VASSERT(dipole != VNULL);
02672     ux = dipole[0];
02673     uy = dipole[1];
02674     uz = dipole[2];
02675     if (quad != VNULL) {
02676         /* The factor of 1/3 results from using a
02677          * traceless quadrupole definition. See, for example,
02678          * "The Theory of Intermolecular Forces" by A.J. Stone,
02679          * Chapter 3. */
02680         qxx = quad[0] / 3.0;
02681         qxy = quad[1] / 3.0;
02682         qxz = quad[2] / 3.0;
02683         qyx = quad[3] / 3.0;
02684         qyy = quad[4] / 3.0;
02685         qyz = quad[5] / 3.0;
02686         qzx = quad[6] / 3.0;
02687         qzy = quad[7] / 3.0;
02688         qzz = quad[8] / 3.0;
02689     } else {
02690         qxx = 0.0;
02691         qxy = 0.0;
02692         qxz = 0.0;
02693         qyx = 0.0;
02694         qyy = 0.0;
02695         qyz = 0.0;
02696         qzx = 0.0;
02697         qzy = 0.0;
02698         qzz = 0.0;
02699     }
02700
02701     pre = (Vunit_ec*Vunit_ec)/(4*VPI*Vunit_eps0*Vunit_kb*T);
02702     pre = pre*(1.0e10);
02703
02704     /* the "i" boundaries (dirichlet) */
02705     for (k=0; k<nz; k++) {
02706         gpos[2] = zf[k];
02707         for (j=0; j<ny; j++) {
02708             gpos[1] = yf[j];
02709             gpos[0] = xf[0];
02710             xr = gpos[0] - apos[0];
02711             yr = gpos[1] - apos[1];
02712             zr = gpos[2] - apos[2];
02713             dist = VSQRT(VSQR(xr) + VSQR(yr) + VSQR(zr));
02714             multipolebc(dist, xkappa, eps_p, eps_w, size, tensor);
02715             val = pre*charge*tensor[0];
02716             val -= pre*ux*xr*tensor[1];
02717             val -= pre*uy*yr*tensor[1];
02718             val -= pre*uz*zr*tensor[1];
02719             val += pre*qxx*xr*xr*tensor[2];
02720             val += pre*qyy*yr*yr*tensor[2];
02721             val += pre*qzz*zr*zr*tensor[2];
02722             val += pre*2.0*qxy*xr*yr*tensor[2];
02723             val += pre*2.0*qxz*xr*zr*tensor[2];
02724             val += pre*2.0*qyz*yr*zr*tensor[2];
02725             gxcf[IJKx(j,k,0)] += val;
02726
02727             gpos[0] = xf[nx-1];
02728             xr = gpos[0] - apos[0];
02729             dist = VSQRT(VSQR(xr) + VSQR(yr) + VSQR(zr));
02730             multipolebc(dist, xkappa, eps_p, eps_w, size, tensor);
02731             val = pre*charge*tensor[0];
02732             val -= pre*ux*xr*tensor[1];
02733             val -= pre*uy*yr*tensor[1];
02734             val -= pre*uz*zr*tensor[1];
02735             val += pre*qxx*xr*xr*tensor[2];
02736             val += pre*qyy*yr*yr*tensor[2];
02737             val += pre*qzz*zr*zr*tensor[2];
02738             val += pre*2.0*qxy*xr*yr*tensor[2];
02739             val += pre*2.0*qxz*xr*zr*tensor[2];
02740             val += pre*2.0*qyz*yr*zr*tensor[2];
02741             gxcf[IJKx(j,k,1)] += val;
02742         }
02743     }
02744
02745     /* the "j" boundaries (dirichlet) */
02746     for (k=0; k<nz; k++) {

```

```

02747     gpos[2] = zf[k];
02748     for (i=0; i<nx; i++) {
02749         gpos[0] = xf[i];
02750         gpos[1] = yf[0];
02751         xr = gpos[0] - apos[0];
02752         yr = gpos[1] - apos[1];
02753         zr = gpos[2] - apos[2];
02754         dist = VSQRT(VSQR(xr) + VSQR(yr) + VSQR(zr));
02755         multipolebc(dist, xkappa, eps_p, eps_w, size, tensor);
02756         val = pre*charge*tensor[0];
02757         val -= pre*ux*xr*tensor[1];
02758         val -= pre*uy*yr*tensor[1];
02759         val -= pre*uz*zr*tensor[1];
02760         val += pre*qxx*xr*xr*tensor[2];
02761         val += pre*qyy*yr*yr*tensor[2];
02762         val += pre*qzz*zr*zr*tensor[2];
02763         val += pre*2.0*qxy*xr*yr*tensor[2];
02764         val += pre*2.0*qxz*xr*zr*tensor[2];
02765         val += pre*2.0*qyz*yr*zr*tensor[2];
02766         gycf[IJKy(i,k,0)] += val;
02767
02768         gpos[1] = yf[ny-1];
02769         yr = gpos[1] - apos[1];
02770         dist = VSQRT(VSQR(xr) + VSQR(yr) + VSQR(zr));
02771         multipolebc(dist, xkappa, eps_p, eps_w, size, tensor);
02772         val = pre*charge*tensor[0];
02773         val -= pre*ux*xr*tensor[1];
02774         val -= pre*uy*yr*tensor[1];
02775         val -= pre*uz*zr*tensor[1];
02776         val += pre*qxx*xr*xr*tensor[2];
02777         val += pre*qyy*yr*yr*tensor[2];
02778         val += pre*qzz*zr*zr*tensor[2];
02779         val += pre*2.0*qxy*xr*yr*tensor[2];
02780         val += pre*2.0*qxz*xr*zr*tensor[2];
02781         val += pre*2.0*qyz*yr*zr*tensor[2];
02782         gycf[IJKy(i,k,1)] += val;
02783     }
02784 }
02785
02786 /* the "k" boundaries (dirichlet) */
02787 for (j=0; j<ny; j++) {
02788     gpos[1] = yf[j];
02789     for (i=0; i<nx; i++) {
02790         gpos[0] = xf[i];
02791         gpos[2] = zf[0];
02792         xr = gpos[0] - apos[0];
02793         yr = gpos[1] - apos[1];
02794         zr = gpos[2] - apos[2];
02795         dist = VSQRT(VSQR(xr) + VSQR(yr) + VSQR(zr));
02796         multipolebc(dist, xkappa, eps_p, eps_w, size, tensor);
02797         val = pre*charge*tensor[0];
02798         val -= pre*ux*xr*tensor[1];
02799         val -= pre*uy*yr*tensor[1];
02800         val -= pre*uz*zr*tensor[1];
02801         val += pre*qxx*xr*xr*tensor[2];
02802         val += pre*qyy*yr*yr*tensor[2];
02803         val += pre*qzz*zr*zr*tensor[2];
02804         val += pre*2.0*qxy*xr*yr*tensor[2];
02805         val += pre*2.0*qxz*xr*zr*tensor[2];
02806         val += pre*2.0*qyz*yr*zr*tensor[2];
02807         gzcfc[IJKz(i,j,0)] += val;
02808
02809         gpos[2] = zf[nz-1];
02810         zr = gpos[2] - apos[2];
02811         dist = VSQRT(VSQR(xr) + VSQR(yr) + VSQR(zr));
02812         multipolebc(dist, xkappa, eps_p, eps_w, size, tensor);
02813         val = pre*charge*tensor[0];
02814         val -= pre*ux*xr*tensor[1];
02815         val -= pre*uy*yr*tensor[1];
02816         val -= pre*uz*zr*tensor[1];
02817         val += pre*qxx*xr*xr*tensor[2];
02818         val += pre*qyy*yr*yr*tensor[2];
02819         val += pre*qzz*zr*zr*tensor[2];
02820         val += pre*2.0*qxy*xr*yr*tensor[2];
02821         val += pre*2.0*qxz*xr*zr*tensor[2];
02822         val += pre*2.0*qyz*yr*zr*tensor[2];
02823         gzcfc[IJKz(i,j,1)] += val;
02824     }
02825 }
02826 }
02827

```



```

02828 VPRIVATE void bcCalcOrig(Vpmg *thee) {
02829
02830     int nx, ny, nz;
02831     double size, *position, charge, xkappa, eps_w, T, prel;
02832     double *dipole, *quadrupole, debye, eps_p;
02833     double xr, yr, zr, qave, *apos;
02834     double sdhcharge, sdhdipole[3], traced[9], sdhquadrupole[9];
02835     int i, j, k, iatom;
02836     Vpbe *pbe;
02837     Vatom *atom;
02838     Valist *alist;
02839
02840     pbe = thee->pbe;
02841     alist = thee->pbe->alist;
02842     nx = thee->pmgp->nx;
02843     ny = thee->pmgp->ny;
02844     nz = thee->pmgp->nz;
02845
02846     /* Zero out the boundaries */
02847     /* the "i" boundaries (dirichlet) */
02848     for (k=0; k<nz; k++) {
02849         for (j=0; j<ny; j++) {
02850             thee->gxcf[IJKx(j,k,0)] = 0.0;
02851             thee->gxcf[IJKx(j,k,1)] = 0.0;
02852             thee->gxcf[IJKx(j,k,2)] = 0.0;
02853             thee->gxcf[IJKx(j,k,3)] = 0.0;
02854         }
02855     }
02856
02857     /* the "j" boundaries (dirichlet) */
02858     for (k=0; k<nz; k++) {
02859         for (i=0; i<nx; i++) {
02860             thee->gycf[IJKy(i,k,0)] = 0.0;
02861             thee->gycf[IJKy(i,k,1)] = 0.0;
02862             thee->gycf[IJKy(i,k,2)] = 0.0;
02863             thee->gycf[IJKy(i,k,3)] = 0.0;
02864         }
02865     }
02866
02867     /* the "k" boundaries (dirichlet) */
02868     for (j=0; j<ny; j++) {
02869         for (i=0; i<nx; i++) {
02870             thee->gzcf[IJKz(i,j,0)] = 0.0;
02871             thee->gzcf[IJKz(i,j,1)] = 0.0;
02872             thee->gzcf[IJKz(i,j,2)] = 0.0;
02873             thee->gzcf[IJKz(i,j,3)] = 0.0;
02874         }
02875     }
02876
02877     /* For each "atom" (only one for bcfl=1), we use the following formula to
02878     * calculate the boundary conditions:
02879     * 
$$g(x) = \frac{q}{4\pi\epsilon_0\epsilon_w k_b T} \frac{\exp(-xkappa(d-a))}{1+xkappa a}$$

02880     * where  $d = ||x - x_0||$  (in m) and  $a$  is the size of the atom (in m).
02881     * We only need to evaluate some of these prefactors once:
02882     *  $prel = \frac{q}{4\pi\epsilon_0\epsilon_w k_b T}$ 
02883     * which gives the potential as
02884     * 
$$g(x) = prel * q/d * \frac{\exp(-xkappa(d-a))}{1+xkappa a}$$

02885     */
02886     eps_w = Vpbe_getSolventDiel(pbe); /* Dimensionless */
02887     eps_p = Vpbe_getSoluteDiel(pbe); /* Dimensionless */
02888     T = Vpbe_getTemperature(pbe); /* K */
02889     prel = (Vunit_ec)/(4*VPI*Vunit_eps0*eps_w*Vunit_kb*T);
02890
02891     /* Finally, if we convert keep xkappa in A-1 and scale prel by
02892     * m/A, then we will only need to deal with distances and sizes in
02893     * Angstroms rather than meters. */
02894     xkappa = Vpbe_getXkappa(pbe); /* A-1 */
02895     prel = prel*(1.0e10);
02896
02897     switch (thee->pmgp->bcfl) {
02898     /* If we have zero boundary conditions, we're done */
02899     case BCFL_ZERO:
02900         return;
02901
02902     /* For single DH sphere BC's, we only have one "atom" to deal with;
02903     * get its information and */
02904     case BCFL_SDH:
02905         size = Vpbe_getSoluteRadius(pbe);
02906         position = Vpbe_getSoluteCenter(pbe);
02907     }

```

```

02909
02910      /*
02911      For AMOEBA SDH boundary conditions, we need to find the
02912      total monopole, dipole and traceless quadrupole moments
02913      of either the permanent multipoles, induced dipoles or
02914      non-local induced dipoles.
02915      */
02916
02917      sdhcharge = 0.0;
02918      for (i=0; i<3; i++) sdhdipole[i] = 0.0;
02919      for (i=0; i<9; i++) sdhquadrupole[i] = 0.0;
02920
02921      for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
02922          atom = Valist_getAtom(alist, iatom);
02923          apos = Vatom_getPosition(atom);
02924          xr = apos[0] - position[0];
02925          yr = apos[1] - position[1];
02926          zr = apos[2] - position[2];
02927          switch (three->chargeSrc) {
02928              case VCM_CHARGE:
02929                  charge = Vatom_getCharge(atom);
02930                  sdhcharge += charge;
02931                  sdhdipole[0] += xr * charge;
02932                  sdhdipole[1] += yr * charge;
02933                  sdhdipole[2] += zr * charge;
02934                  traced[0] = xr*xr*charge;
02935                  traced[1] = xr*yr*charge;
02936                  traced[2] = xr*zr*charge;
02937                  traced[3] = yr*xr*charge;
02938                  traced[4] = yr*yr*charge;
02939                  traced[5] = yr*zr*charge;
02940                  traced[6] = zr*xr*charge;
02941                  traced[7] = zr*yr*charge;
02942                  traced[8] = zr*zr*charge;
02943                  qave = (traced[0] + traced[4] + traced[8]) / 3.0;
02944                  sdhquadrupole[0] += 1.5*(traced[0] - qave);
02945                  sdhquadrupole[1] += 1.5*(traced[1]);
02946                  sdhquadrupole[2] += 1.5*(traced[2]);
02947                  sdhquadrupole[3] += 1.5*(traced[3]);
02948                  sdhquadrupole[4] += 1.5*(traced[4] - qave);
02949                  sdhquadrupole[5] += 1.5*(traced[5]);
02950                  sdhquadrupole[6] += 1.5*(traced[6]);
02951                  sdhquadrupole[7] += 1.5*(traced[7]);
02952                  sdhquadrupole[8] += 1.5*(traced[8] - qave);
02953          #if defined(WITH_TINKER)
02954              case VCM_PERMANENT:
02955                  charge = Vatom_getCharge(atom);
02956                  dipole = Vatom_getDipole(atom);
02957                  quadrupole = Vatom_getQuadrupole(atom);
02958                  sdhcharge += charge;
02959                  sdhdipole[0] += xr * charge;
02960                  sdhdipole[1] += yr * charge;
02961                  sdhdipole[2] += zr * charge;
02962                  traced[0] = xr*xr*charge;
02963                  traced[1] = xr*yr*charge;
02964                  traced[2] = xr*zr*charge;
02965                  traced[3] = yr*xr*charge;
02966                  traced[4] = yr*yr*charge;
02967                  traced[5] = yr*zr*charge;
02968                  traced[6] = zr*xr*charge;
02969                  traced[7] = zr*yr*charge;
02970                  traced[8] = zr*zr*charge;
02971                  sdhdipole[0] += dipole[0];
02972                  sdhdipole[1] += dipole[1];
02973                  sdhdipole[2] += dipole[2];
02974                  traced[0] += 2.0*xr*dipole[0];
02975                  traced[1] += xr*dipole[1] + yr*dipole[0];
02976                  traced[2] += xr*dipole[2] + zr*dipole[0];
02977                  traced[3] += yr*dipole[0] + xr*dipole[1];
02978                  traced[4] += 2.0*yr*dipole[1];
02979                  traced[5] += yr*dipole[2] + zr*dipole[1];
02980                  traced[6] += zr*dipole[0] + xr*dipole[2];
02981                  traced[7] += zr*dipole[1] + yr*dipole[2];
02982                  traced[8] += 2.0*zr*dipole[2];
02983                  qave = (traced[0] + traced[4] + traced[8]) / 3.0;
02984                  sdhquadrupole[0] += 1.5*(traced[0] - qave);
02985                  sdhquadrupole[1] += 1.5*(traced[1]);
02986                  sdhquadrupole[2] += 1.5*(traced[2]);
02987                  sdhquadrupole[3] += 1.5*(traced[3]);
02988                  sdhquadrupole[4] += 1.5*(traced[4] - qave);
02989                  sdhquadrupole[5] += 1.5*(traced[5]);

```

```

02990         sdhquadrupole[6] += 1.5*(traced[6]);
02991         sdhquadrupole[7] += 1.5*(traced[7]);
02992         sdhquadrupole[8] += 1.5*(traced[8] - qave);
02993         sdhquadrupole[0] += quadrupole[0];
02994         sdhquadrupole[1] += quadrupole[1];
02995         sdhquadrupole[2] += quadrupole[2];
02996         sdhquadrupole[3] += quadrupole[3];
02997         sdhquadrupole[4] += quadrupole[4];
02998         sdhquadrupole[5] += quadrupole[5];
02999         sdhquadrupole[6] += quadrupole[6];
03000         sdhquadrupole[7] += quadrupole[7];
03001         sdhquadrupole[8] += quadrupole[8];
03002     case VCM_INDUCED:
03003         dipole = Vatom_getInducedDipole(atom);
03004         sdhdipole[0] += dipole[0];
03005         sdhdipole[1] += dipole[1];
03006         sdhdipole[2] += dipole[2];
03007         traced[0] = 2.0*xr*dipole[0];
03008         traced[1] = xr*dipole[1] + yr*dipole[0];
03009         traced[2] = xr*dipole[2] + zr*dipole[0];
03010         traced[3] = yr*dipole[0] + xr*dipole[1];
03011         traced[4] = 2.0*yr*dipole[1];
03012         traced[5] = yr*dipole[2] + zr*dipole[1];
03013         traced[6] = zr*dipole[0] + xr*dipole[2];
03014         traced[7] = zr*dipole[1] + yr*dipole[2];
03015         traced[8] = 2.0*zr*dipole[2];
03016         qave = (traced[0] + traced[4] + traced[8]) / 3.0;
03017         sdhquadrupole[0] += 1.5*(traced[0] - qave);
03018         sdhquadrupole[1] += 1.5*(traced[1]);
03019         sdhquadrupole[2] += 1.5*(traced[2]);
03020         sdhquadrupole[3] += 1.5*(traced[3]);
03021         sdhquadrupole[4] += 1.5*(traced[4] - qave);
03022         sdhquadrupole[5] += 1.5*(traced[5]);
03023         sdhquadrupole[6] += 1.5*(traced[6]);
03024         sdhquadrupole[7] += 1.5*(traced[7]);
03025         sdhquadrupole[8] += 1.5*(traced[8] - qave);
03026     case VCM_NLINDUCED:
03027         dipole = Vatom_getNLInducedDipole(atom);
03028         sdhdipole[0] += dipole[0];
03029         sdhdipole[1] += dipole[1];
03030         sdhdipole[2] += dipole[2];
03031         traced[0] = 2.0*xr*dipole[0];
03032         traced[1] = xr*dipole[1] + yr*dipole[0];
03033         traced[2] = xr*dipole[2] + zr*dipole[0];
03034         traced[3] = yr*dipole[0] + xr*dipole[1];
03035         traced[4] = 2.0*yr*dipole[1];
03036         traced[5] = yr*dipole[2] + zr*dipole[1];
03037         traced[6] = zr*dipole[0] + xr*dipole[2];
03038         traced[7] = zr*dipole[1] + yr*dipole[2];
03039         traced[8] = 2.0*zr*dipole[2];
03040         qave = (traced[0] + traced[4] + traced[8]) / 3.0;
03041         sdhquadrupole[0] += 1.5*(traced[0] - qave);
03042         sdhquadrupole[1] += 1.5*(traced[1]);
03043         sdhquadrupole[2] += 1.5*(traced[2]);
03044         sdhquadrupole[3] += 1.5*(traced[3]);
03045         sdhquadrupole[4] += 1.5*(traced[4] - qave);
03046         sdhquadrupole[5] += 1.5*(traced[5]);
03047         sdhquadrupole[6] += 1.5*(traced[6]);
03048         sdhquadrupole[7] += 1.5*(traced[7]);
03049         sdhquadrupole[8] += 1.5*(traced[8] - qave);
03050         /*Added the else to kill a warning when building with clang*/
03051     #else
03052         case VCM_PERMANENT;;
03053         case VCM_INDUCED;;
03054         case VCM_NLINDUCED;;
03055     #endif /* if defined(WITH_TINKER) */
03056     }
03057 }
03058 /* SDH dipole and traceless quadrupole values
03059 were checked against similar routines in TINKER
03060 for large proteins.
03061
03062 debye=4.8033324;
03063 printf("%6.3f, %6.3f, %6.3f\n", sdhdipole[0]*debye,
03064 sdhdipole[1]*debye, sdhdipole[2]*debye);
03065 printf("%6.3f\n", sdhquadrupole[0]*debye);
03066 printf("%6.3f %6.3f\n", sdhquadrupole[3]*debye,
03067 sdhquadrupole[4]*debye);
03068 printf("%6.3f %6.3f %6.3f\n", sdhquadrupole[6]*debye,
03069 sdhquadrupole[7]*debye, sdhquadrupole[8]*debye);
03070 */

```

```

03071
03072         bcfl2(size, position, sdhcharge, sdhdipole, sdhquadrupole,
03073             xkappa, eps_p, eps_w, T, thee->gxcf, thee->gycf,
03074             thee->gzcf, thee->xf, thee->yf, thee->zf, nx, ny, nz);
03075         break;
03076
03077     case BCFL_MDH:
03078         for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
03079             atom = Valist_getAtom(alist, iatom);
03080             position = Vatom_getPosition(atom);
03081             charge = Vunit_ec*Vatom_getCharge(atom);
03082             dipole = VNULL;
03083             quadrupole = VNULL;
03084             size = Vatom_getRadius(atom);
03085             switch (thee->chargeSrc)
03086             {
03087                 case VCM_CHARGE:
03088                     ;
03089             #if defined(WITH_TINKER)
03090                 case VCM_PERMANENT:
03091                     dipole = Vatom_getDipole(atom);
03092                     quadrupole = Vatom_getQuadrupole(atom);
03093
03094                 case VCM_INDUCED:
03095                     dipole = Vatom_getInducedDipole(atom);
03096
03097                 case VCM_NLINDUCED:
03098                     dipole = Vatom_getNLInducedDipole(atom);
03099             /*added this to kill a warning when building with clang (by Juan Brandi).*/
03100             #else
03101                 case VCM_PERMANENT;;
03102                 case VCM_INDUCED;;
03103                 case VCM_NLINDUCED;;
03104             #endif
03105             }
03106             bcfl1(size, position, charge, xkappa, prel,
03107                 thee->gxcf, thee->gycf, thee->gzcf,
03108                 thee->xf, thee->yf, thee->zf, nx, ny, nz);
03109         }
03110         break;
03111
03112     case BCFL_UNUSED:
03113         Vnm_print(2, "bcCalc: Invalid bcfl (%d)!\n", thee->pmgp->bcfl);
03114         VASSERT(0);
03115
03116     case BCFL_FOCUS:
03117         Vnm_print(2, "VPMG::bcCalc -- not appropriate for focusing!\n");
03118         VASSERT(0);
03119
03120     default:
03121         Vnm_print(2, "VPMG::bcCalc -- invalid boundary condition \
03122 flag (%d)!\n", thee->pmgp->bcfl);
03123         VASSERT(0);
03124     }
03125 }
03126
03127 /*
03128 Used by bcflnew
03129 */
03130 VPRIVATE int gridPointIsValid(int i, int j, int k, int nx, int ny, int nz){
03131
03132     int isValid = 0;
03133
03134     if ((k==0) || (k==nz-1)){
03135         isValid = 1;
03136     }else if ((j==0) || (j==ny-1)){
03137         isValid = 1;
03138     }else if ((i==0) || (i==nx-1)){
03139         isValid = 1;
03140     }
03141
03142     return isValid;
03143 }
03144
03145 /*
03146 Used by bcflnew
03147 */
03148 #ifdef DEBUG_MAC_OSX_OCL
03149 #include "mach_chud.h"
03150 VPRIVATE void packAtomsOpenCL(float *ax, float *ay, float *az,
03151                             float *charge, float *size, Vpmg *thee){

```

```

03152
03153     int i;
03154     int natoms;
03155
03156     Vatom *atom = VNULL;
03157     Valist *alist = VNULL;
03158
03159     alist = thee->pbe->alist;
03160     natoms = Valist_getNumberAtoms(alist);
03161
03162     for(i=0;i<natoms;i++){
03163         atom = &(alist->atoms[i]);
03164         charge[i] = Vunit_ec*atom->charge;
03165         ax[i] = atom->position[0];
03166         ay[i] = atom->position[1];
03167         az[i] = atom->position[2];
03168         size[i] = atom->radius;
03169     }
03170 }
03171
03172 /*
03173 Used by bcfnew
03174 */
03175 VPRIVATE void packUnpackOpenCL(int nx, int ny, int nz, int ngrid,
03176                                float *gx, float *gy, float *gz, float *value,
03177                                Vpmg *thee, int pack){
03178
03179     int i,j,k,igrid;
03180     int x0,x1,y0,y1,z0,z1;
03181
03182     float gpos[3];
03183     double *xf, *yf, *zf;
03184     double *gxcf, *gycf, *gzcf;
03185
03186     xf = thee->xf;
03187     yf = thee->yf;
03188     zf = thee->zf;
03189
03190     gxcf = thee->gxcf;
03191     gycf = thee->gycf;
03192     gzcf = thee->gzcf;
03193
03194     igrid = 0;
03195     for(k=0;k<nz;k++){
03196         gpos[2] = zf[k];
03197         for(j=0;j<ny;j++){
03198             gpos[1] = yf[j];
03199             for(i=0;i<nx;i++){
03200                 gpos[0] = xf[i];
03201                 if(gridPointIsValid(i, j, k, nx, ny, nz)){
03202                     if(pack != 0){
03203                         gx[igrid] = gpos[0];
03204                         gy[igrid] = gpos[1];
03205                         gz[igrid] = gpos[2];
03206
03207                         value[igrid] = 0.0;
03208                     }else{
03209                         x0 = IJKx(j,k,0);
03210                         x1 = IJKx(j,k,1);
03211                         y0 = IJKy(i,k,0);
03212                         y1 = IJKy(i,k,1);
03213                         z0 = IJKz(i,j,0);
03214                         z1 = IJKz(i,j,1);
03215
03216                         if(i==0){
03217                             gxcf[x0] += value[igrid];
03218                         }
03219                         if(i==nx-1){
03220                             gxcf[x1] += value[igrid];
03221                         }
03222                         if(j==0){
03223                             gycf[y0] += value[igrid];
03224                         }
03225                         if(j==ny-1){
03226                             gycf[y1] += value[igrid];
03227                         }
03228                         if(k==0){
03229                             gzcf[z0] += value[igrid];
03230                         }
03231                         if(k==nz-1){
03232                             gzcf[z1] += value[igrid];
03233

```

```

03233         }
03234     }
03235
03236         igrid++;
03237     } //end is valid point
03238 } //end i
03239 } //end j
03240 } //end k
03241
03242 }
03243
03244 /*
03245 bcflnew is an optimized replacement for bcfl1. bcfl1 is still used when TINKER
03246 support is compiled in.
03247 bcflnew uses: packUnpack, packAtoms, gridPointIsValid
03248 */
03249 VPRIVATE void bcflnewOpenCL(Vpmg *thee){
03250
03251     int i,j,k, iatom, igrid;
03252     int x0, x1, y0, y1, z0, z1;
03253
03254     int nx, ny, nz;
03255     int natoms, ngrid, ngadj;
03256
03257     float dist, prel, eps_w, eps_p, T, xkappa;
03258
03259     float *ax, *ay, *az;
03260     float *charge, *size, *val;
03261
03262     float *gx, *gy, *gz;
03263
03264     Vpbe *pbe = thee->pbe;
03265
03266     nx = thee->pmgp->nx;
03267     ny = thee->pmgp->ny;
03268     nz = thee->pmgp->nz;
03269
03270     eps_w = Vpbe_getSolventDiel(pbe);          /* Dimensionless */
03271     eps_p = Vpbe_getSoluteDiel(pbe);           /* Dimensionless */
03272     T = Vpbe_getTemperature(pbe);              /* K */
03273     prel = ((Vunit_ec)/(4*VPI*Vunit_eps0*eps_w*Vunit_kb*T))*(1.0e10);
03274     xkappa = Vpbe_getXkappa(pbe);
03275
03276     natoms = Valist_getNumberAtoms(thee->pbe->alist);
03277     ngrid = 2*((nx*ny) + (ny*nz) + (nx*nz));
03278     ngadj = ngrid + (512 - (ngrid & 511));
03279
03280     ax = (float*)malloc(natoms * sizeof(float));
03281     ay = (float*)malloc(natoms * sizeof(float));
03282     az = (float*)malloc(natoms * sizeof(float));
03283
03284     charge = (float*)malloc(natoms * sizeof(float));
03285     size = (float*)malloc(natoms * sizeof(float));
03286
03287     gx = (float*)malloc(ngrid * sizeof(float));
03288     gy = (float*)malloc(ngrid * sizeof(float));
03289     gz = (float*)malloc(ngrid * sizeof(float));
03290
03291     val = (float*)malloc(ngrid * sizeof(float));
03292
03293     packAtomsOpenCL(ax, ay, az, charge, size, thee);
03294     packUnpackOpenCL(nx, ny, nz, ngrid, gx, gy, gz, val, thee, 1);
03295
03296     runMDHCL(ngrid, natoms, ngadj, ax, ay, az, gx, gy, gz, charge, size, xkappa, prel, val);
03297
03298     packUnpackOpenCL(nx, ny, nz, ngrid, gx, gy, gz, val, thee, 0);
03299
03300     free(ax);
03301     free(ay);
03302     free(az);
03303     free(charge);
03304     free(size);
03305
03306     free(gx);
03307     free(gy);
03308     free(gz);
03309     free(val);
03310 }
03311 #endif
03312
03313 VPRIVATE void packAtoms(double *ax, double *ay, double *az,

```

```

03314         double *charge, double *size, Vpmg *thee){
03315
03316     int i;
03317     int natoms;
03318
03319     Vatom *atom = VNULL;
03320     Valist *alist = VNULL;
03321
03322     alist = thee->pbe->alist;
03323     natoms = Valist_getNumberAtoms(alist);
03324
03325     for(i=0;i<natoms;i++){
03326         atom = &(alist->atoms[i]);
03327         charge[i] = Vunit_ec*atom->charge;
03328         ax[i] = atom->position[0];
03329         ay[i] = atom->position[1];
03330         az[i] = atom->position[2];
03331         size[i] = atom->radius;
03332     }
03333 }
03334
03335 /*
03336 Used by bcflnew
03337 */
03338 VPRIVATE void packUnpack(int nx, int ny, int nz, int ngrid,
03339     double *gx, double *gy, double *gz, double *value,
03340     Vpmg *thee, int pack){
03341
03342     int i,j,k,igrid;
03343     int x0,x1,y0,y1,z0,z1;
03344
03345     double gpos[3];
03346     double *xf, *yf, *zf;
03347     double *gxcf, *gycf, *gzcf;
03348
03349     xf = thee->xf;
03350     yf = thee->yf;
03351     zf = thee->zf;
03352
03353     gxcf = thee->gxcf;
03354     gycf = thee->gycf;
03355     gzcf = thee->gzcf;
03356
03357     igrid = 0;
03358     for(k=0;k<nz;k++){
03359         gpos[2] = zf[k];
03360         for(j=0;j<ny;j++){
03361             gpos[1] = yf[j];
03362             for(i=0;i<nx;i++){
03363                 gpos[0] = xf[i];
03364                 if(gridPointIsValid(i, j, k, nx, ny, nz)){
03365                     if(pack != 0){
03366                         gx[igrid] = gpos[0];
03367                         gy[igrid] = gpos[1];
03368                         gz[igrid] = gpos[2];
03369
03370                         value[igrid] = 0.0;
03371                     }else{
03372                         x0 = IJKx(j,k,0);
03373                         x1 = IJKx(j,k,1);
03374                         y0 = IJKy(i,k,0);
03375                         y1 = IJKy(i,k,1);
03376                         z0 = IJKz(i,j,0);
03377                         z1 = IJKz(i,j,1);
03378
03379                         if(i==0){
03380                             gxcf[x0] += value[igrid];
03381                         }
03382                         if(i==nx-1){
03383                             gxcf[x1] += value[igrid];
03384                         }
03385                         if(j==0){
03386                             gycf[y0] += value[igrid];
03387                         }
03388                         if(j==ny-1){
03389                             gycf[y1] += value[igrid];
03390                         }
03391                         if(k==0){
03392                             gzcf[z0] += value[igrid];
03393                         }
03394                         if(k==nz-1){

```

```

03395             gzcf[z1] += value[igrid];
03396         }
03397     }
03398     igrid++;
03400 } //end is valid point
03401 } //end i
03402 } //end j
03403 } //end k
03404 }
03405 }
03406
03407 VPRIVATE void bcflnew(Vpmg *thee){
03408     int i,j,k, iatom, igrid;
03410     int x0, x1, y0, y1, z0, z1;
03411
03412     int nx, ny, nz;
03413     int natoms, ngrid;
03414
03415     double dist, prel, eps_w, eps_p, T, xkappa;
03416
03417     double *ax, *ay, *az;
03418     double *charge, *size, *val;
03419
03420     double *gx, *gy, *gz;
03421
03422     Vpbe *pbe = thee->pbe;
03423
03424     nx = thee->pmgp->nx;
03425     ny = thee->pmgp->ny;
03426     nz = thee->pmgp->nz;
03427
03428     eps_w = Vpbe_getSolventDiel(pbe);           /* Dimensionless */
03429     eps_p = Vpbe_getSoluteDiel(pbe);           /* Dimensionless */
03430     T = Vpbe_getTemperature(pbe);             /* K */
03431     prel = ((Vunit_ec)/(4*VPI*Vunit_eps0*eps_w*Vunit_kb*T))*(1.0e10);
03432     xkappa = Vpbe_getXkappa(pbe);
03433
03434     natoms = Valist_getNumberAtoms(thee->pbe->alist);
03435     ngrid = 2*((nx*ny) + (ny*nz) + (nx*nz));
03436
03437     ax = (double*)malloc(natoms * sizeof(double));
03438     ay = (double*)malloc(natoms * sizeof(double));
03439     az = (double*)malloc(natoms * sizeof(double));
03440
03441     charge = (double*)malloc(natoms * sizeof(double));
03442     size = (double*)malloc(natoms * sizeof(double));
03443
03444     gx = (double*)malloc(ngrid * sizeof(double));
03445     gy = (double*)malloc(ngrid * sizeof(double));
03446     gz = (double*)malloc(ngrid * sizeof(double));
03447
03448     val = (double*)malloc(ngrid * sizeof(double));
03449
03450     packAtoms(ax,ay,az,charge,size,thee);
03451     packUnpack(nx,ny,nz,ngrid,gx,gy,gz,val,thee,1);
03452
03453     if(xkappa > VSMALL){
03454 #pragma omp parallel for default(shared) private(igrid,iatom,dist)
03455         for(igrid=0;igrid<ngrid;igrid++){
03456             for(iatom=0; iatom<natoms; iatom++){
03457                 dist = VSQRT(VSQR(gx[igrid]-ax[iatom]) + VSQR(gy[igrid]-ay[iatom])
03458                     + VSQR(gz[igrid]-az[iatom]));
03459                 val[igrid] += prel*(charge[iatom]/dist)*VEXP(-xkappa*(dist-size[iatom]))
03460                     / (1+xkappa*size[iatom]);
03461             }
03462         }
03463     }else{
03464 #pragma omp parallel for default(shared) private(igrid,iatom,dist)
03465         for(igrid=0;igrid<ngrid;igrid++){
03466             for(iatom=0; iatom<natoms; iatom++){
03467                 dist = VSQRT(VSQR(gx[igrid]-ax[iatom]) + VSQR(gy[igrid]-ay[iatom])
03468                     + VSQR(gz[igrid]-az[iatom]));
03469                 val[igrid] += prel*(charge[iatom]/dist);
03470             }
03471         }
03472     }
03473     packUnpack(nx,ny,nz,ngrid,gx,gy,gz,val,thee,0);
03474
03475     free(ax);

```



```

03476     free(ay);
03477     free(az);
03478     free(charge);
03479     free(size);
03480
03481     free(gx);
03482     free(gy);
03483     free(gz);
03484     free(val);
03485 }
03486
03487 VPRIVATE void multipolebc(double r, double kappa, double eps_p,
03488                          double eps_w, double rad, double tsr[3]) {
03489     double r2,r3,r5;
03490     double eps_r;
03491     double ka,ka2,ka3;
03492     double kr,kr2,kr3;
03493
03494     /*
03495     Below an attempt is made to explain the potential outside of a
03496     multipole located at the center of spherical cavity of dielectric
03497     eps_p, with dielectric eps_w outside (and possibly kappa > 0).
03498
03499     First, eps_p = 1.0
03500     eps_w = 1.0
03501     kappa = 0.0
03502
03503     The general form for the potential of a traceless multipole tensor
03504     of rank n in vacuum is:
03505
03506     
$$V(r) = (-1)^n \cdot u \cdot \nabla^n (1/r)$$

03507
03508     where
03509     u                is a multipole of order n (3^n components)
03510     u · ∇n (1/r)    is the contraction of u with the nth
03511     derivative of 1/r
03512
03513     for example, if n = 1, the dipole potential is
03514     
$$V_{vac}(r) = (-1) \cdot [u_x \cdot x + u_y \cdot y + u_z \cdot z] / r^3$$

03515
03516     This function returns the parts of V(r) for multipoles of
03517     order 0, 1 and 2 that are independent of the contraction.
03518
03519     For the vacuum example, this would be 1/r, -1/r^3 and 3/r^5
03520     respectively.
03521
03522     *** Note that this requires that the quadrupole is
03523     traceless. If not, the diagonal quadrupole potential changes
03524     from
03525     qaa * 3*a^2/r^5
03526     to
03527     qaa * (3*a^2/r^5 - 1/r^3a )
03528     where we sum over the trace; a = x, y and z.
03529
03530     (In other words, the -1/r^3 term cancels for a traceless quadrupole.
03531     qxx + qyy + qzz = 0
03532     such that
03533     -(qxx + qyy + qzz)/r^3 = 0
03534
03535     For quadrupole with trace:
03536     qxx + qyy + qzz != 0
03537     such that
03538     -(qxx + qyy + qzz)/r^3 != 0
03539     )
03540
03541     =====
03542
03543     eps_p != 1 or eps_w != 1
03544     kappa = 0.0
03545
03546     If the multipole is placed at the center of a sphere with
03547     dielectric eps_p in a solvent of dielectric eps_w, the potential
03548     outside the sphere is the solution to the Laplace equation:
03549
03550     
$$V(r) = 1/\epsilon_w \cdot (2n+1) \cdot \epsilon_r / (n(n+1) \cdot \epsilon_p) \cdot$$

03551     * (-1)^n * u · ∇n (1/r)
03552     where
03553     eps_r = eps_w / eps_p
03554     is the ratio of solvent to solute dielectric
03555
03556

```

```

03557  =====
03558
03559  kappa > 0
03560
03561  Finally, if the region outside the sphere is treated by the linearized
03562  PB equation with Debye-Huckel parameter kappa, the solution is:
03563
03564  V(r) = kappa/eps_w * alpha_n(kappa*a) * K_n(kappa*r) * r^(n+1)/a^n
03565  * (-1)^n * u . n . Del^n (1/r)
03566  where
03567  alpha_n(x) is [(2n + 1) / x] / [(n*K_n(x)/eps_r) - x*K_n'(x)]
03568  K_n(x) are modified spherical Bessel functions of the third kind.
03569  K_n'(x) is the derivative of K_n(x)
03570  */
03571
03572  eps_r = eps_w/eps_p;
03573  r2 = r*r;
03574  r3 = r2*r;
03575  r5 = r3*r2;
03576  tsr[0] = (1.0/eps_w)/r;
03577  tsr[1] = (1.0/eps_w)*(-1.0)/r3;
03578  tsr[2] = (1.0/eps_w)*(3.0)/r5;
03579  if (kappa < VSMALL) {
03580      tsr[1] = (3.0*eps_r)/(1.0 + 2.0*eps_r)*tsr[1];
03581      tsr[2] = (5.0*eps_r)/(2.0 + 3.0*eps_r)*tsr[2];
03582  } else {
03583      ka = kappa*rad;
03584      ka2 = ka*ka;
03585      ka3 = ka2*ka;
03586      kr = kappa*r;
03587      kr2 = kr*kr;
03588      kr3 = kr2*kr;
03589      tsr[0] = exp(ka-kr) / (1.0 + ka) * tsr[0];
03590      tsr[1] = 3.0*eps_r*exp(ka-kr)*(1.0 + kr) * tsr[1];
03591      tsr[1] = tsr[1] / (1.0 + ka + eps_r*(2.0 + 2.0*ka + ka2));
03592      tsr[2] = 5.0*eps_r*exp(ka-kr)*(3.0 + 3.0*kr + kr2) * tsr[2];
03593      tsr[2] = tsr[2]/(6.0+6.0*ka+2.0*ka2+eps_r*(9.0+9.0*ka+4.0*ka2+ka3));
03594  }
03595 }
03596
03597 VPRIVATE void bcfl_sdh(Vpmg *thee) {
03598
03599     int i,j,k,iatom;
03600     int nx, ny, nz;
03601
03602     double size, *position, charge, xkappa, eps_w, eps_p, T, pre, dist;
03603     double sdhcharge, sdhdipole[3], traced[9], sdhquadrupole[9];
03604     double *dipole, *quadrupole;
03605
03606     double val, *apos, gpos[3], tensor[3], qave;
03607     double ux, uy, uz, xr, yr, zr;
03608     double qxx,qxy,qxz,qyx,qyy,qyz,qzx,qzy,qzz;
03609
03610     double *xf, *yf, *zf;
03611     double *gxcf, *gycf, *gzcf;
03612
03613     Vpbe *pbe;
03614     Vatom *atom;
03615     Valist *alist;
03616
03617     pbe = thee->pbe;
03618     alist = thee->pbe->alist;
03619     nx = thee->pmgp->nx;
03620     ny = thee->pmgp->ny;
03621     nz = thee->pmgp->nz;
03622
03623     xf = thee->xf;
03624     yf = thee->yf;
03625     zf = thee->zf;
03626
03627     gxcf = thee->gxcf;
03628     gycf = thee->gycf;
03629     gzcf = thee->gzcf;
03630
03631     /* For each "atom" (only one for bcfl=1), we use the following formula to
03632     * calculate the boundary conditions:
03633     *   g(x) = \frac{q e_c}{4*\pi*\eps_0*\eps_w*k_b*T}
03634     *         * \frac{\exp(-xkappa*(d - a))}{1+xkappa*a}
03635     *         * 1/d
03636     * where d = ||x - x_0|| (in m) and a is the size of the atom (in m).
03637     * We only need to evaluate some of these prefactors once:

```

```

03638      *   prel = \frac{e_c}{4*\pi*\epsilon_0*\epsilon_w*k_b*T}
03639      *   which gives the potential as
03640      *   g(x) = prel * q/d * \frac{\exp(-xkappa*(d - a))}{1+xkappa*a}
03641      */
03642     eps_w = Vpbe_getSolventDiel(pbe);           /* Dimensionless */
03643     eps_p = Vpbe_getSoluteDiel(pbe);           /* Dimensionless */
03644     T = Vpbe_getTemperature(pbe);              /* K */
03645
03646     pre = (Vunit_ec*Vunit_ec)/(4*VPI*Vunit_eps0*Vunit_kb*T);
03647     pre = pre*(1.0e10);
03648
03649     /* Finally, if we convert keep xkappa in A^{-1} and scale prel by
03650      * m/A, then we will only need to deal with distances and sizes in
03651      * Angstroms rather than meters. */
03652     xkappa = Vpbe_getXkappa(pbe);              /* A^{-1} */
03653
03654     /* Solute size and position */
03655     size = Vpbe_getSoluteRadius(pbe);
03656     position = Vpbe_getSoluteCenter(pbe);
03657
03658     sdhcharge = 0.0;
03659     for (i=0; i<3; i++) sdhdipole[i] = 0.0;
03660     for (i=0; i<9; i++) sdhquadrupole[i] = 0.0;
03661
03662     for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
03663         atom = Valist_getAtom(alist, iatom);
03664         apos = Vatom_getPosition(atom);
03665         xr = apos[0] - position[0];
03666         yr = apos[1] - position[1];
03667         zr = apos[2] - position[2];
03668         switch (three->chargeSrc) {
03669             case VCM_CHARGE:
03670                 charge = Vatom_getCharge(atom);
03671                 sdhcharge += charge;
03672                 sdhdipole[0] += xr * charge;
03673                 sdhdipole[1] += yr * charge;
03674                 sdhdipole[2] += zr * charge;
03675                 traced[0] = xr*xr*charge;
03676                 traced[1] = xr*yr*charge;
03677                 traced[2] = xr*zr*charge;
03678                 traced[3] = yr*xr*charge;
03679                 traced[4] = yr*yr*charge;
03680                 traced[5] = yr*zr*charge;
03681                 traced[6] = zr*xr*charge;
03682                 traced[7] = zr*yr*charge;
03683                 traced[8] = zr*zr*charge;
03684                 qave = (traced[0] + traced[4] + traced[8]) / 3.0;
03685                 sdhquadrupole[0] += 1.5*(traced[0] - qave);
03686                 sdhquadrupole[1] += 1.5*(traced[1]);
03687                 sdhquadrupole[2] += 1.5*(traced[2]);
03688                 sdhquadrupole[3] += 1.5*(traced[3]);
03689                 sdhquadrupole[4] += 1.5*(traced[4] - qave);
03690                 sdhquadrupole[5] += 1.5*(traced[5]);
03691                 sdhquadrupole[6] += 1.5*(traced[6]);
03692                 sdhquadrupole[7] += 1.5*(traced[7]);
03693                 sdhquadrupole[8] += 1.5*(traced[8] - qave);
03694             #if defined(WITH_TINKER)
03695                 case VCM_PERMANENT:
03696                     charge = Vatom_getCharge(atom);
03697                     dipole = Vatom_getDipole(atom);
03698                     quadrupole = Vatom_getQuadrupole(atom);
03699                     sdhcharge += charge;
03700                     sdhdipole[0] += xr * charge;
03701                     sdhdipole[1] += yr * charge;
03702                     sdhdipole[2] += zr * charge;
03703                     traced[0] = xr*xr*charge;
03704                     traced[1] = xr*yr*charge;
03705                     traced[2] = xr*zr*charge;
03706                     traced[3] = yr*xr*charge;
03707                     traced[4] = yr*yr*charge;
03708                     traced[5] = yr*zr*charge;
03709                     traced[6] = zr*xr*charge;
03710                     traced[7] = zr*yr*charge;
03711                     traced[8] = zr*zr*charge;
03712                     sdhdipole[0] += dipole[0];
03713                     sdhdipole[1] += dipole[1];
03714                     sdhdipole[2] += dipole[2];
03715                     traced[0] += 2.0*xr*dipole[0];
03716                     traced[1] += xr*dipole[1] + yr*dipole[0];
03717                     traced[2] += xr*dipole[2] + zr*dipole[0];
03718                     traced[3] += yr*dipole[0] + xr*dipole[1];

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```

03719         traced[4] += 2.0*yr*dipole[1];
03720         traced[5] += yr*dipole[2] + zr*dipole[1];
03721         traced[6] += zr*dipole[0] + xr*dipole[2];
03722         traced[7] += zr*dipole[1] + yr*dipole[2];
03723         traced[8] += 2.0*zr*dipole[2];
03724         gave = (traced[0] + traced[4] + traced[8]) / 3.0;
03725         sdhquadrupole[0] += 1.5*(traced[0] - gave);
03726         sdhquadrupole[1] += 1.5*(traced[1]);
03727         sdhquadrupole[2] += 1.5*(traced[2]);
03728         sdhquadrupole[3] += 1.5*(traced[3]);
03729         sdhquadrupole[4] += 1.5*(traced[4] - gave);
03730         sdhquadrupole[5] += 1.5*(traced[5]);
03731         sdhquadrupole[6] += 1.5*(traced[6]);
03732         sdhquadrupole[7] += 1.5*(traced[7]);
03733         sdhquadrupole[8] += 1.5*(traced[8] - gave);
03734         sdhquadrupole[0] += quadrupole[0];
03735         sdhquadrupole[1] += quadrupole[1];
03736         sdhquadrupole[2] += quadrupole[2];
03737         sdhquadrupole[3] += quadrupole[3];
03738         sdhquadrupole[4] += quadrupole[4];
03739         sdhquadrupole[5] += quadrupole[5];
03740         sdhquadrupole[6] += quadrupole[6];
03741         sdhquadrupole[7] += quadrupole[7];
03742         sdhquadrupole[8] += quadrupole[8];
03743     case VCM_INDUCED:
03744         dipole = Vatom_getInducedDipole(atom);
03745         sdhdipole[0] += dipole[0];
03746         sdhdipole[1] += dipole[1];
03747         sdhdipole[2] += dipole[2];
03748         traced[0] = 2.0*xr*dipole[0];
03749         traced[1] = xr*dipole[1] + yr*dipole[0];
03750         traced[2] = xr*dipole[2] + zr*dipole[0];
03751         traced[3] = yr*dipole[0] + xr*dipole[1];
03752         traced[4] = 2.0*yr*dipole[1];
03753         traced[5] = yr*dipole[2] + zr*dipole[1];
03754         traced[6] = zr*dipole[0] + xr*dipole[2];
03755         traced[7] = zr*dipole[1] + yr*dipole[2];
03756         traced[8] = 2.0*zr*dipole[2];
03757         gave = (traced[0] + traced[4] + traced[8]) / 3.0;
03758         sdhquadrupole[0] += 1.5*(traced[0] - gave);
03759         sdhquadrupole[1] += 1.5*(traced[1]);
03760         sdhquadrupole[2] += 1.5*(traced[2]);
03761         sdhquadrupole[3] += 1.5*(traced[3]);
03762         sdhquadrupole[4] += 1.5*(traced[4] - gave);
03763         sdhquadrupole[5] += 1.5*(traced[5]);
03764         sdhquadrupole[6] += 1.5*(traced[6]);
03765         sdhquadrupole[7] += 1.5*(traced[7]);
03766         sdhquadrupole[8] += 1.5*(traced[8] - gave);
03767     case VCM_NLINDUCED:
03768         dipole = Vatom_getNLInducedDipole(atom);
03769         sdhdipole[0] += dipole[0];
03770         sdhdipole[1] += dipole[1];
03771         sdhdipole[2] += dipole[2];
03772         traced[0] = 2.0*xr*dipole[0];
03773         traced[1] = xr*dipole[1] + yr*dipole[0];
03774         traced[2] = xr*dipole[2] + zr*dipole[0];
03775         traced[3] = yr*dipole[0] + xr*dipole[1];
03776         traced[4] = 2.0*yr*dipole[1];
03777         traced[5] = yr*dipole[2] + zr*dipole[1];
03778         traced[6] = zr*dipole[0] + xr*dipole[2];
03779         traced[7] = zr*dipole[1] + yr*dipole[2];
03780         traced[8] = 2.0*zr*dipole[2];
03781         gave = (traced[0] + traced[4] + traced[8]) / 3.0;
03782         sdhquadrupole[0] += 1.5*(traced[0] - gave);
03783         sdhquadrupole[1] += 1.5*(traced[1]);
03784         sdhquadrupole[2] += 1.5*(traced[2]);
03785         sdhquadrupole[3] += 1.5*(traced[3]);
03786         sdhquadrupole[4] += 1.5*(traced[4] - gave);
03787         sdhquadrupole[5] += 1.5*(traced[5]);
03788         sdhquadrupole[6] += 1.5*(traced[6]);
03789         sdhquadrupole[7] += 1.5*(traced[7]);
03790         sdhquadrupole[8] += 1.5*(traced[8] - gave);
03791     /*added this to kill a warning when building with clang (by Juan Brandi)*/
03792     #else
03793         case VCM_PERMANENT;;
03794         case VCM_INDUCED;;
03795         case VCM_NLINDUCED;;
03796     #endif /* if defined(WITH_TINKER) */
03797     }
03798 }
03799

```

```

03800     ux = sdhdipole[0];
03801     uy = sdhdipole[1];
03802     uz = sdhdipole[2];
03803
03804     /* The factor of 1/3 results from using a
03805     traceless quadrupole definition. See, for example,
03806     "The Theory of Intermolecular Forces" by A.J. Stone,
03807     Chapter 3. */
03808     qxx = sdhquadrupole[0] / 3.0;
03809     qxy = sdhquadrupole[1] / 3.0;
03810     qxz = sdhquadrupole[2] / 3.0;
03811     qyx = sdhquadrupole[3] / 3.0;
03812     qyy = sdhquadrupole[4] / 3.0;
03813     qyz = sdhquadrupole[5] / 3.0;
03814     qzx = sdhquadrupole[6] / 3.0;
03815     qzy = sdhquadrupole[7] / 3.0;
03816     qzz = sdhquadrupole[8] / 3.0;
03817
03818     for(k=0; k<nz; k++){
03819         gpos[2] = zf[k];
03820         for(j=0; j<ny; j++){
03821             gpos[1] = yf[j];
03822             for(i=0; i<nx; i++){
03823                 gpos[0] = xf[i];
03824                 if(gridPointIsValid(i, j, k, nx, ny, nz)){
03825                     xr = gpos[0] - position[0];
03826                     yr = gpos[1] - position[1];
03827                     zr = gpos[2] - position[2];
03828
03829                     dist = VSQR(VSQR(xr) + VSQR(yr) + VSQR(zr));
03830                     multipolebc(dist, xkappa, eps_p, eps_w, size, tensor);
03831
03832                     val = pre*sdhcharge*tensor[0];
03833                     val -= pre*ux*xr*tensor[1];
03834                     val -= pre*uy*yr*tensor[1];
03835                     val -= pre*uz*zr*tensor[1];
03836                     val += pre*qxx*xr*xr*tensor[2];
03837                     val += pre*qyy*yr*yr*tensor[2];
03838                     val += pre*qzz*zr*zr*tensor[2];
03839                     val += pre*2.0*qxy*xr*yr*tensor[2];
03840                     val += pre*2.0*qxz*xr*zr*tensor[2];
03841                     val += pre*2.0*qyz*yr*zr*tensor[2];
03842
03843                     if(i==0){
03844                         gxcf[IJKx(j,k,0)] = val;
03845                     }
03846                     if(i==nx-1){
03847                         gxcf[IJKx(j,k,1)] = val;
03848                     }
03849                     if(j==0){
03850                         gycf[IJKy(i,k,0)] = val;
03851                     }
03852                     if(j==ny-1){
03853                         gycf[IJKy(i,k,1)] = val;
03854                     }
03855                     if(k==0){
03856                         gzcf[IJKz(i,j,0)] = val;
03857                     }
03858                     if(k==nz-1){
03859                         gzcf[IJKz(i,j,1)] = val;
03860                     }
03861                 } /* End grid point is valid */
03862             } /* End i loop */
03863         } /* End j loop */
03864     } /* End k loop */
03865
03866 }
03867
03868 VPRIVATE void bcf1_mdh(Vpmg *thee){
03869
03870     int i,j,k,iatom;
03871     int nx, ny, nz;
03872
03873     double val, *apos, gpos[3];
03874     double *dipole, *quadrupole;
03875     double size, charge, xkappa, eps_w, eps_p, T, prel, dist;
03876
03877     double *xf, *yf, *zf;
03878     double *gxcf, *gycf, *gzcf;
03879
03880     Vpbe *pbe;

```

```

03881     Vatom *atom;
03882     Valist *alist;
03883
03884     pbe = thee->pbe;
03885     alist = thee->pbe->alist;
03886     nx = thee->pmgpp->nx;
03887     ny = thee->pmgpp->ny;
03888     nz = thee->pmgpp->nz;
03889
03890     xf = thee->xf;
03891     yf = thee->yf;
03892     zf = thee->zf;
03893
03894     gxcf = thee->gxcf;
03895     gycf = thee->gycf;
03896     gzcf = thee->gzcf;
03897
03898     /* For each "atom" (only one for bcfl=1), we use the following formula to
03899      * calculate the boundary conditions:
03900      * 
$$g(x) = \frac{q e_c}{4\pi\epsilon_0\epsilon_w k_b T} \frac{\exp(-\kappa(d-a))}{1+\kappa a}$$

03901      * where  $d = ||x - x_0||$  (in m) and  $a$  is the size of the atom (in m).
03902      * We only need to evaluate some of these prefactors once:
03903      *  $prel = \frac{e_c}{4\pi\epsilon_0\epsilon_w k_b T}$ 
03904      * which gives the potential as
03905      * 
$$g(x) = prel * q/d * \frac{\exp(-\kappa(d-a))}{1+\kappa a}$$

03906      */
03907     eps_w = Vpbe_getSolventDiel(pbe); /* Dimensionless */
03908     eps_p = Vpbe_getSoluteDiel(pbe); /* Dimensionless */
03909     T = Vpbe_getTemperature(pbe); /* K */
03910     prel = (Vunit_ec)/(4*VPI*Vunit_eps0*eps_w*Vunit_kb*T);
03911
03912     /* Finally, if we convert keep  $\kappa$  in  $\text{\AA}^{-1}$  and scale  $prel$  by
03913      * m/ $\text{\AA}$ , then we will only need to deal with distances and sizes in
03914      * Angstroms rather than meters. */
03915     kappa = Vpbe_getXkappa(pbe); /*  $\text{\AA}^{-1}$  */
03916     prel = prel*(1.0e10);
03917
03918     /* Finally, if we convert keep  $\kappa$  in  $\text{\AA}^{-1}$  and scale  $prel$  by
03919      * m/ $\text{\AA}$ , then we will only need to deal with distances and sizes in
03920      * Angstroms rather than meters. */
03921     kappa = Vpbe_getXkappa(pbe); /*  $\text{\AA}^{-1}$  */
03922
03923     for(k=0;k<nz;k++){
03924         gpos[2] = zf[k];
03925         for(j=0;j<ny;j++){
03926             gpos[1] = yf[j];
03927             for(i=0;i<nx;i++){
03928                 gpos[0] = xf[i];
03929                 if(gridPointIsValid(i, j, k, nx, ny, nz)){
03930                     val = 0.0;
03931
03932                     for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
03933                         atom = Valist_getAtom(alist, iatom);
03934                         apos = Vatom_getPosition(atom);
03935                         charge = Vunit_ec*Vatom_getCharge(atom);
03936                         size = Vatom_getRadius(atom);
03937
03938                         dist = VSQR(VSQR(gpos[0]-apos[0]) + VSQR(gpos[1]-apos[1])
03939                                     + VSQR(gpos[2]-apos[2]));
03940                         if (kappa > VSMALL) {
03941                             val += prel*(charge/dist)*VEXP(-kappa*(dist-size))
03942                                     / (1+kappa*size);
03943                         } else {
03944                             val += prel*(charge/dist);
03945                         }
03946                     }
03947
03948                     if(i==0){
03949                         gxcf[IJKx(j,k,0)] = val;
03950                     }
03951                     if(i==nx-1){
03952                         gxcf[IJKx(j,k,1)] = val;
03953                     }
03954                     if(j==0){
03955                         gycf[IJKy(i,k,0)] = val;
03956                     }
03957                     if(j==ny-1){
03958

```

```

03962         gycf[IJKy(i,k,1)] = val;
03963     }
03964     if(k==0){
03965         gzcfc[IJKz(i,j,0)] = val;
03966     }
03967     if(k==nz-1){
03968         gzcfc[IJKz(i,j,1)] = val;
03969     }
03970     } /* End grid point is valid */
03971 } /* End i loop */
03972 } /* End j loop */
03973 } /* End k loop */
03974
03975 }
03976
03977 /* ////////////////////////////////////////
03978 // Routine:  bcfl_mem
03979 //
03980 // Purpose:  Increment all the boundary points by the
03981 //           analytic expression for a membrane system in
03982 //           the presence of a membrane potential. This
03983 //           Boundary flag should only be used for systems
03984 //           that explicitly have membranes in the dielectric
03985 //           and solvent maps.
03986 //
03987 //           There should be several input variables add to this
03988 //           function such as membrane potential, membrane thickness
03989 //           and height.
03990 //
03991 // Args:     apos is a 3-vector
03992 //
03993 // Author:   Michael Grabe
03994 VPRIVATE void bcfl_mem(double zmem, double L, double eps_m, double eps_w,
03995 double V, double xkappa, double *gxcfc, double *gycfc, double *gzcfc,
03996 double *xf, double *yf, double *zf, int nx, int ny, int nz) {
03997
04000     /* some definitions */
04001     /* L = total length of the membrane */
04002     /* xkappa = inverse Debye length */
04003     /* zmem = z value of membrane bottom (Cytoplasm) */
04004     /* V = electrical potential inside the cell */
04005     int i, j, k;
04006     double dist, val, z_low, z_high, z_shift;
04007     double A, B, C, D, edge_L, l;
04008     double G, z_0, z_rel;
04009     double gpos[3];
04010
04011     Vnm_print(0, "Here is the value of kappa: %f\n",xkappa);
04012     Vnm_print(0, "Here is the value of L: %f\n",L);
04013     Vnm_print(0, "Here is the value of zmem: %f\n",zmem);
04014     Vnm_print(0, "Here is the value of mdie: %f\n",eps_m);
04015     Vnm_print(0, "Here is the value of memv: %f\n",V);
04016
04017     /* no salt symmetric BC's at +/- infinity */
04018     // B=V/(edge_L - l*(1-eps_w/eps_m));
04019     // A=V + B*edge_L;
04020     // D=eps_w/eps_m*B;
04021     z_low = zmem; /* this defines the bottom of the membrane */
04022     z_high = zmem + L; /* this is the top of the membrane */
04023
04024     /*
04025     //*****
04026     // proper boundary conditions for V = 0 extracellular */
04027     // and psi=-V cytoplasm. */
04028     // Implicit in this formulation is that the membrane */
04029     // center be at z = 0 */
04030     //*****
04031
04032     l=L/2; /* half of the membrane length */
04033     z_0 = z_low + l; /* center of the membrane */
04034     G=l*eps_w/eps_m*xkappa;
04035     A=-V/2*(1/(G+1))*exp(xkappa*l);
04036     B=V/2;
04037     C=-V/2*eps_w/eps_m*xkappa*(1/(G+1));
04038     D=-A;
04039     /* The analytic expression for the boundary conditions */
04040     /* had the cytoplasmic surface of the membrane set to zero. */
04041     /* This requires an off-set of the BC equations. */
04042
04043     /* the "i" boundaries (dirichlet) */
04044     for (k=0; k<nz; k++) {
04045         gpos[2] = zf[k];

```

```

04046     z_rel = gpos[2] - z_0;    /* relative position for BCs */
04047
04048     for (j=0; j<ny; j++) {
04049
04050         if (gpos[2] <= z_low) {                                /* cytoplasmic */
04051
04052             val = A*exp(xkappa*z_rel) + V;
04053             gxcf[IJKx(j,k,0)] += val;    /* assign low side BC */
04054             gxcf[IJKx(j,k,1)] += val;    /* assign high side BC */
04055
04056         }
04057
04058         else if (gpos[2] > z_low && gpos[2] <= z_high) {    /* in membrane */
04059
04060             val = B + C*z_rel;
04061             gxcf[IJKx(j,k,0)] += val;    /* assign low side BC */
04062             gxcf[IJKx(j,k,1)] += val;    /* assign high side BC */
04063
04064         }
04065
04066         else if (gpos[2] > z_high) {                            /* extracellular */
04067
04068             val = D*exp(-xkappa*z_rel);
04069             gxcf[IJKx(j,k,0)] += val;    /* assign low side BC */
04070             gxcf[IJKx(j,k,1)] += val;    /* assign high side BC */
04071
04072         }
04073
04074     }
04075 }
04076
04077 /* the "j" boundaries (dirichlet) */
04078 for (k=0; k<nz; k++) {
04079     gpos[2] = zf[k];
04080     z_rel = gpos[2] - z_0;
04081     for (i=0; i<nix; i++) {
04082
04083         if (gpos[2] <= z_low) {                                /* cytoplasmic */
04084
04085             val = A*exp(xkappa*z_rel) + V;
04086             gycf[IJKy(i,k,0)] += val;    /* assign low side BC */
04087             gycf[IJKy(i,k,1)] += val;    /* assign high side BC */
04088             //printf("%f \n",val);
04089
04090         }
04091
04092         else if (gpos[2] > z_low && gpos[2] <= z_high) {    /* in membrane */
04093
04094             val = B + C*z_rel;
04095             gycf[IJKy(i,k,0)] += val;    /* assign low side BC */
04096             gycf[IJKy(i,k,1)] += val;    /* assign high side BC */
04097             //printf("%f \n",val);
04098
04099         }
04100         else if (gpos[2] > z_high) {                            /* extracellular */
04101
04102             val = D*exp(-xkappa*z_rel);
04103             gycf[IJKy(i,k,0)] += val;    /* assign low side BC */
04104             gycf[IJKy(i,k,1)] += val;    /* assign high side BC */
04105             //printf("%f \n",val);
04106
04107         }
04108
04109     }
04110 }
04111
04112 /* the "k" boundaries (dirichlet) */
04113 for (j=0; j<ny; j++) {
04114     for (i=0; i<nix; i++) {
04115
04116         /* first assign the bottom boundary */
04117
04118         gpos[2] = zf[0];
04119         z_rel = gpos[2] - z_0;
04120
04121         if (gpos[2] <= z_low) {                                /* cytoplasmic */
04122
04123             val = A*exp(xkappa*z_rel) + V;
04124             gzc[IJKz(i,j,0)] += val;    /* assign low side BC */
04125             //printf("%f \n",val);
04126

```



```

04127     }
04128
04129     else if (gpos[2] > z_low && gpos[2] <= z_high) { /* in membrane */
04130
04131         val = B + C*z_rel;
04132         gzcf[IJKz(i,j,0)] += val; /* assign low side BC */
04133     }
04134
04135     else if (gpos[2] > z_high) { /* extracellular */
04136
04137         val = D*exp(-xkappa*z_rel);
04138         gzcf[IJKz(i,j,0)] += val; /* assign low side BC */
04139     }
04140
04141     /* now assign the top boundary */
04142
04143     gpos[2] = zf[nz-1];
04144     z_rel = gpos[2] - z_0;
04145
04146     if (gpos[2] <= z_low) { /* cytoplasmic */
04147
04148         val = A*exp(xkappa*z_rel) + V;
04149         gzcf[IJKz(i,j,1)] += val; /* assign high side BC */
04150     }
04151
04152     else if (gpos[2] > z_low && gpos[2] <= z_high) { /* in membrane */
04153
04154         val = B + C*z_rel;
04155         gzcf[IJKz(i,j,1)] += val; /* assign high side BC */
04156     }
04157
04158     else if (gpos[2] > z_high) { /* extracellular */
04159
04160         val = D*exp(-xkappa*z_rel);
04161         gzcf[IJKz(i,j,1)] += val; /* assign high side BC */
04162         //printf("%f \n",val);
04163     }
04164 }
04165 }
04166 }
04167 }
04168 }
04169 }
04170 }
04171 }
04172 }
04173
04174 VPRIVATE void bcfl_map(Vpmg *thee){
04175
04176     Vpbe *pbe;
04177     double position[3], pot, hx, hy, hzed;
04178     int i, j, k, nx, ny, nz, rc;
04179
04180
04181     VASSERT(thee != VNULL);
04182
04183     /* Mesh info */
04184     nx = thee->pmgp->nx;
04185     ny = thee->pmgp->ny;
04186     nz = thee->pmgp->nz;
04187     hx = thee->pmgp->hx;
04188     hy = thee->pmgp->hy;
04189     hzed = thee->pmgp->hzed;
04190
04191     /* Reset the potential array */
04192     for (i=0; i<(nx*ny*nz); i++) thee->pot[i] = 0.0;
04193
04194     /* Fill in the source term (atomic potentials) */
04195     Vnm_print(0, "Vpmg_fillco: filling in source term.\n");
04196     for (k=0; k<nz; k++) {
04197         for (j=0; j<ny; j++) {
04198             for (i=0; i<nx; i++) {
04199                 position[0] = thee->xf[i];
04200                 position[1] = thee->yf[j];
04201                 position[2] = thee->zf[k];
04202                 rc = Vgrid_value(thee->potMap, position, &pot);
04203                 if (!rc) {
04204                     Vnm_print(2, "fillcoChargeMap: Error -- fell off of potential map at (%g, %g,
04205 %g)!\n",
04206                             position[0], position[1], position[2]);
04207                     VASSERT(0);
04208                 }
04209             }
04210         }
04211     }

```

```

04207         }
04208         thee->pot[IJK(i,j,k)] = pot;
04209     }
04210 }
04211 }
04212
04213 }
04214
04215 #if defined(WITH_TINKER)
04216 VPRIVATE void bcf1_mdh_tinker(Vpmg *thee){
04217
04218     int i,j,k,iatom;
04219     int nx, ny, nz;
04220
04221     double val, *apos, gpos[3], tensor[9];
04222     double *dipole, *quadrupole;
04223     double size, charge, xkappa, eps_w, eps_p, T, prel, dist;
04224
04225     double ux,uy,uz,xr,yr,zr;
04226     double qxx,qxy,qxz,qyx,qyy,qyz,qzx,qzy,qzz;
04227
04228     double *xf, *yf, *zf;
04229     double *gxcf, *gycf, *gzcf;
04230
04231     Vpbe *pbe;
04232     Vatom *atom;
04233     Valist *alist;
04234
04235     pbe = thee->pbe;
04236     alist = thee->pbe->alist;
04237     nx = thee->pmgp->nx;
04238     ny = thee->pmgp->ny;
04239     nz = thee->pmgp->nz;
04240
04241     xf = thee->xf;
04242     yf = thee->yf;
04243     zf = thee->zf;
04244
04245     gxcf = thee->gxcf;
04246     gycf = thee->gycf;
04247     gzcf = thee->gzcf;
04248
04249     /* For each "atom" (only one for bcf1=1), we use the following formula to
04250      * calculate the boundary conditions:
04251      * 
$$g(x) = \frac{q}{4\pi\epsilon_0\epsilon_w k_b T} \frac{\exp(-xkappa(d-a))}{1+xkappa a}$$

04252      * where  $d = ||x - x_0||$  (in m) and  $a$  is the size of the atom (in m).
04253      * We only need to evaluate some of these prefactors once:
04254      *  $prel = \frac{q}{4\pi\epsilon_0\epsilon_w k_b T}$ 
04255      * which gives the potential as
04256      *  $g(x) = prel * q/d * \frac{\exp(-xkappa(d-a))}{1+xkappa a}$ 
04257      */
04258     eps_w = Vpbe_getSolventDiel(pbe); /* Dimensionless */
04259     eps_p = Vpbe_getSoluteDiel(pbe); /* Dimensionless */
04260     T = Vpbe_getTemperature(pbe); /* K */
04261     prel = (Vunit_ec*Vunit_ec)/(4*VPI*Vunit_eps0*Vunit_kb*T);
04262
04263     /* Finally, if we convert keep xkappa in A-1 and scale prel by
04264      * m/A, then we will only need to deal with distances and sizes in
04265      * Angstroms rather than meters. */
04266     xkappa = Vpbe_getXkappa(pbe); /* A-1 */
04267     prel = prel*(1.0e10);
04268
04269     /* Finally, if we convert keep xkappa in A-1 and scale prel by
04270      * m/A, then we will only need to deal with distances and sizes in
04271      * Angstroms rather than meters. */
04272     xkappa = Vpbe_getXkappa(pbe); /* A-1 */
04273
04274     for(k=0;k<nz;k++){
04275         gpos[2] = zf[k];
04276         for(j=0;j<ny;j++){
04277             gpos[1] = yf[j];
04278             for(i=0;i<nx;i++){
04279                 gpos[0] = xf[i];
04280                 if(gridPointIsValid(i, j, k, nx, ny, nz)){
04281                     val = 0.0;
04282
04283                     for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
04284                         atom = Valist_getAtom(alist, iatom);

```

```

04288         apos = Vatom_getPosition(atom);
04289         size = Vatom_getRadius(atom);
04290
04291         charge = 0.0;
04292
04293         dipole = VNULL;
04294         quadrupole = VNULL;
04295
04296         if (thee->chargeSrc == VCM_PERMANENT) {
04297             charge = Vatom_getCharge(atom);
04298             dipole = Vatom_getDipole(atom);
04299             quadrupole = Vatom_getQuadrupole(atom);
04300         } else if (thee->chargeSrc == VCM_INDUCED) {
04301             dipole = Vatom_getInducedDipole(atom);
04302         } else {
04303             dipole = Vatom_getNLInducedDipole(atom);
04304         }
04305
04306         ux = dipole[0];
04307         uy = dipole[1];
04308         uz = dipole[2];
04309
04310         if (quadrupole != VNULL) {
04311             /* The factor of 1/3 results from using a
04312              * traceless quadrupole definition. See, for example,
04313              * "The Theory of Intermolecular Forces" by A.J. Stone,
04314              * Chapter 3. */
04315             qxx = quadrupole[0] / 3.0;
04316             qxy = quadrupole[1] / 3.0;
04317             qxz = quadrupole[2] / 3.0;
04318             qyx = quadrupole[3] / 3.0;
04319             qyy = quadrupole[4] / 3.0;
04320             qyz = quadrupole[5] / 3.0;
04321             qzx = quadrupole[6] / 3.0;
04322             qzy = quadrupole[7] / 3.0;
04323             qzz = quadrupole[8] / 3.0;
04324         } else {
04325             qxx = 0.0;
04326             qxy = 0.0;
04327             qxz = 0.0;
04328             qyx = 0.0;
04329             qyy = 0.0;
04330             qyz = 0.0;
04331             qzx = 0.0;
04332             qzy = 0.0;
04333             qzz = 0.0;
04334         }
04335
04336         xr = gpos[0] - apos[0];
04337         yr = gpos[1] - apos[1];
04338         zr = gpos[2] - apos[2];
04339
04340         dist = VSQRT(VSQR(xr) + VSQR(yr) + VSQR(zr));
04341         multipolebc(dist, xkappa, eps_p, eps_w, size, tensor);
04342
04343         val += prel*charge*tensor[0];
04344         val -= prel*ux*xr*tensor[1];
04345         val -= prel*uy*yr*tensor[1];
04346         val -= prel*uz*zr*tensor[1];
04347         val += prel*qxx*xr*xr*tensor[2];
04348         val += prel*qyy*yr*yr*tensor[2];
04349         val += prel*qzz*zr*zr*tensor[2];
04350         val += prel*2.0*qxy*xr*yr*tensor[2];
04351         val += prel*2.0*qxz*xr*zr*tensor[2];
04352         val += prel*2.0*qyz*yr*zr*tensor[2];
04353
04354     }
04355
04356     if (i==0) {
04357         gxcf[IJKx(j,k,0)] = val;
04358     }
04359     if (i==nx-1) {
04360         gxcf[IJKx(j,k,1)] = val;
04361     }
04362     if (j==0) {
04363         gycf[IJKy(i,k,0)] = val;
04364     }
04365     if (j==ny-1) {
04366         gycf[IJKy(i,k,1)] = val;
04367     }
04368     if (k==0) {

```

```

04369             gzcf[IJKz(i,j,0)] = val;
04370         }
04371         if(k==nz-1){
04372             gzcf[IJKz(i,j,1)] = val;
04373         }
04374     } /* End grid point is valid */
04375 } /* End i loop */
04376 } /* End j loop */
04377 } /* End k loop */
04378
04379 }
04380 #endif
04381
04382 VPRIVATE void bcCalc(Vpmgp *thee){
04383     int i, j, k;
04384     int nx, ny, nz;
04385
04386     double zmem, eps_m, Lmem, memv, eps_w, xkappa;
04387
04388     nx = thee->pmgp->nx;
04389     ny = thee->pmgp->ny;
04390     nz = thee->pmgp->nz;
04391
04392     /* Zero out the boundaries */
04393     /* the "i" boundaries (dirichlet) */
04394     for (k=0; k<nz; k++) {
04395         for (j=0; j<ny; j++) {
04396             thee->gxcf[IJKx(j,k,0)] = 0.0;
04397             thee->gxcf[IJKx(j,k,1)] = 0.0;
04398             thee->gxcf[IJKx(j,k,2)] = 0.0;
04399             thee->gxcf[IJKx(j,k,3)] = 0.0;
04400         }
04401     }
04402
04403     /* the "j" boundaries (dirichlet) */
04404     for (k=0; k<nz; k++) {
04405         for (i=0; i<nx; i++) {
04406             thee->gycf[IJKy(i,k,0)] = 0.0;
04407             thee->gycf[IJKy(i,k,1)] = 0.0;
04408             thee->gycf[IJKy(i,k,2)] = 0.0;
04409             thee->gycf[IJKy(i,k,3)] = 0.0;
04410         }
04411     }
04412
04413     /* the "k" boundaries (dirichlet) */
04414     for (j=0; j<ny; j++) {
04415         for (i=0; i<nx; i++) {
04416             thee->gzcf[IJKz(i,j,0)] = 0.0;
04417             thee->gzcf[IJKz(i,j,1)] = 0.0;
04418             thee->gzcf[IJKz(i,j,2)] = 0.0;
04419             thee->gzcf[IJKz(i,j,3)] = 0.0;
04420         }
04421     }
04422
04423     switch (thee->pmgp->bcfl) {
04424         /* If we have zero boundary conditions, we're done */
04425         case BCFL_ZERO:
04426             return;
04427         case BCFL_SDH:
04428             bcfl_sdh(thee);
04429             break;
04430         case BCFL_MDH:
04431             #if defined(WITH_TINKER)
04432                 bcfl_mdh_tinker(thee);
04433             #else
04434                 uint64_t mbeg = mach_absolute_time();
04435
04436                 /*
04437                  * If OpenCL is available we use it, otherwise fall back to
04438                  * normal route (CPU multithreaded w/ OpenMP)
04439                  */
04440                 if (kOpenCLAvailable == 1) bcflnewOpenCL(thee);
04441                 else bcflnew(thee);
04442
04443                 mets_(&mbeg, "MDH");
04444             #endif
04445         /* bcfl_mdh(thee); */
04446     }

```

```

04450         bcflnew(thee);
04451 #endif /* DEBUG_MAC_OSX_OCL */
04452
04453 #endif /* WITH_TINKER */
04454         break;
04455     case BCFL_MEM:
04456
04457         zmem = Vpbe_getzmem(thee->pbe);
04458         Lmem = Vpbe_getLmem(thee->pbe);
04459         eps_m = Vpbe_getmembraneDiel(thee->pbe);
04460         memv = Vpbe_getmemv(thee->pbe);
04461
04462         eps_w = Vpbe_getSolventDiel(thee->pbe);
04463         xkappa = Vpbe_getXkappa(thee->pbe);
04464
04465         bcfl_mem(zmem, Lmem, eps_m, eps_w, memv, xkappa,
04466             thee->gxcf, thee->gycf, thee->gzcf,
04467             thee->xf, thee->yf, thee->zf, nx, ny, nz);
04468         break;
04469     case BCFL_UNUSED:
04470         Vnm_print(2, "bcCalc: Invalid bcfl (%d)!\n", thee->pmgp->bcfl);
04471         VASSERT(0);
04472         break;
04473     case BCFL_FOCUS:
04474         Vnm_print(2, "VPMG::bcCalc -- not appropriate for focusing!\n");
04475         VASSERT(0);
04476         break;
04477     case BCFL_MAP:
04478         bcfl_map(thee);
04479         focusFillBound(thee, VNULL);
04480         break;
04481     default:
04482         Vnm_print(2, "VPMG::bcCalc -- invalid boundary condition \
04483             flag (%d)!\n", thee->pmgp->bcfl);
04484         VASSERT(0);
04485         break;
04486     }
04487 }
04488
04489 PRIVATE void fillcoCoefMap(Vpmg *thee) {
04490     Vpbe *pbe;
04491     double ionstr, position[3], tkappa, eps, pot, hx, hy, hzed;
04492     int i, j, k, nx, ny, nz;
04493     double kappamax;
04494     VASSERT(thee != VNULL);
04495
04496     /* Get PBE info */
04497     pbe = thee->pbe;
04498     ionstr = Vpbe_getBulkIonicStrength(pbe);
04499
04500     /* Mesh info */
04501     nx = thee->pmgp->nx;
04502     ny = thee->pmgp->ny;
04503     nz = thee->pmgp->nz;
04504     hx = thee->pmgp->hx;
04505     hy = thee->pmgp->hy;
04506     hzed = thee->pmgp->hzed;
04507
04508     if ((!thee->useDielXMap) || (!thee->useDielYMap)
04509         || (!thee->useDielZMap) || (!thee->useKappaMap) && (ionstr > VPMGSMALL))) {
04510
04511         Vnm_print(2, "fillcoCoefMap: You need to use all coefficient maps!\n");
04512         VASSERT(0);
04513     }
04514
04515     /* Scale the kappa map to values between 0 and 1
04516     Thus get the maximum value in the map - this
04517     is theoretically unnecessary, but a good check.*/
04518     kappamax = -1.00;
04519     for (k=0; k<nz; k++) {
04520         for (j=0; j<ny; j++) {
04521             for (i=0; i<nx; i++) {
04522                 if (ionstr > VPMGSMALL) {
04523                     position[0] = thee->xf[i];
04524                     position[1] = thee->yf[j];
04525                     position[2] = thee->zf[k];
04526                     if (!Vgrid_value(thee->kappaMap, position, &tkappa)) {
04527                         Vnm_print(2, "Vpmg_fillco: Off kappaMap at:\n");
04528                         Vnm_print(2, "Vpmg_fillco: (x,y,z) = (%g,%g,%g)\n",

```

```

04531         position[0], position[1], position[2]);
04532         VASSERT(0);
04533     }
04534     if (tkappa > kappamax) {
04535         kappamax = tkappa;
04536     }
04537     if (tkappa < 0.0){
04538         Vnm_print(2, "Vpmg_fillcoCoefMap: Kappa map less than 0\n");
04539         Vnm_print(2, "Vpmg_fillcoCoefMap: at (x,y,z) = (%g,%g %g)\n",
04540             position[0], position[1], position[2]);
04541         VASSERT(0);
04542     }
04543 }
04544 }
04545 }
04546 }
04547 }
04548 if (kappamax > 1.0){
04549     Vnm_print(2, "Vpmg_fillcoCoefMap: Maximum Kappa value\n");
04550     Vnm_print(2, "%g is greater than 1 - will scale appropriately!\n",
04551         kappamax);
04552 }
04553 else {
04554     kappamax = 1.0;
04555 }
04556
04557 for (k=0; k<nz; k++) {
04558     for (j=0; j<ny; j++) {
04559         for (i=0; i<nx; i++) {
04560
04561             if (ionstr > VPMGSMALL) {
04562                 position[0] = thee->xf[i];
04563                 position[1] = thee->yf[j];
04564                 position[2] = thee->zf[k];
04565                 if (!Vgrid_value(thee->kappaMap, position, &tkappa)) {
04566                     Vnm_print(2, "Vpmg_fillco: Off kappaMap at:\n");
04567                     Vnm_print(2, "Vpmg_fillco: (x,y,z) = (%g,%g %g)\n",
04568                         position[0], position[1], position[2]);
04569                     VASSERT(0);
04570                 }
04571                 if (tkappa < VPMGSMALL) tkappa = 0.0;
04572                 thee->kappa[IJK(i,j,k)] = (tkappa / kappamax);
04573             }
04574
04575             position[0] = thee->xf[i] + 0.5*hx;
04576             position[1] = thee->yf[j];
04577             position[2] = thee->zf[k];
04578             if (!Vgrid_value(thee->dielXMap, position, &eps)) {
04579                 Vnm_print(2, "Vpmg_fillco: Off dielXMap at:\n");
04580                 Vnm_print(2, "Vpmg_fillco: (x,y,z) = (%g,%g %g)\n",
04581                     position[0], position[1], position[2]);
04582                 VASSERT(0);
04583             }
04584             thee->epsx[IJK(i,j,k)] = eps;
04585
04586             position[0] = thee->xf[i];
04587             position[1] = thee->yf[j] + 0.5*hy;
04588             position[2] = thee->zf[k];
04589             if (!Vgrid_value(thee->dielYMap, position, &eps)) {
04590                 Vnm_print(2, "Vpmg_fillco: Off dielYMap at:\n");
04591                 Vnm_print(2, "Vpmg_fillco: (x,y,z) = (%g,%g %g)\n",
04592                     position[0], position[1], position[2]);
04593                 VASSERT(0);
04594             }
04595             thee->epsy[IJK(i,j,k)] = eps;
04596
04597             position[0] = thee->xf[i];
04598             position[1] = thee->yf[j];
04599             position[2] = thee->zf[k] + 0.5*hzed;
04600             if (!Vgrid_value(thee->dielZMap, position, &eps)) {
04601                 Vnm_print(2, "Vpmg_fillco: Off dielZMap at:\n");
04602                 Vnm_print(2, "Vpmg_fillco: (x,y,z) = (%g,%g %g)\n",
04603                     position[0], position[1], position[2]);
04604                 VASSERT(0);
04605             }
04606             thee->epsz[IJK(i,j,k)] = eps;
04607         }
04608     }
04609 }
04610 }
04611

```

```

04612 VPRIVATE void fillcoCoefMol(Vpmg *thee) {
04613
04614     if (thee->useDielXMap || thee->useDielYMap || thee->useDielZMap ||
04615         thee->useKappaMap) {
04616
04617         fillcoCoefMap(thee);
04618
04619     } else {
04620
04621         fillcoCoefMolDiel(thee);
04622         fillcoCoefMolIon(thee);
04623
04624     }
04625 }
04626
04627 VPRIVATE void fillcoCoefMolIon(Vpmg *thee) {
04628
04629     Vacc *acc;
04630     Valist *alist;
04631     Vpbe *pbe;
04632     Vatom *atom;
04633     double xmin, xmax, ymin, ymax, zmin, zmax, ionmask, ionstr;
04634     double xlen, ylen, zlen, irad;
04635     double hx, hy, hzed, *apos, arad;
04636     int i, nx, ny, nz, iatom;
04637     Vsurf_Meth surfMeth;
04638
04639     VASSERT(thee != VNULL);
04640     surfMeth = thee->surfMeth;
04641
04642     /* Get PBE info */
04643     pbe = thee->pbe;
04644     acc = pbe->acc;
04645     alist = pbe->alist;
04646     irad = Vpbe_getMaxIonRadius(pbe);
04647     ionstr = Vpbe_getBulkIonicStrength(pbe);
04648
04649     /* Mesh info */
04650     nx = thee->pmgp->nx;
04651     ny = thee->pmgp->ny;
04652     nz = thee->pmgp->nz;
04653     hx = thee->pmgp->hx;
04654     hy = thee->pmgp->hy;
04655     hzed = thee->pmgp->hzed;
04656
04657     /* Define the total domain size */
04658     xlen = thee->pmgp->xlen;
04659     ylen = thee->pmgp->ylen;
04660     zlen = thee->pmgp->zlen;
04661
04662     /* Define the min/max dimensions */
04663     xmin = thee->pmgp->xcent - (xlen/2.0);
04664     ymin = thee->pmgp->ycent - (ylen/2.0);
04665     zmin = thee->pmgp->zcent - (zlen/2.0);
04666     xmax = thee->pmgp->xcent + (xlen/2.0);
04667     ymax = thee->pmgp->ycent + (ylen/2.0);
04668     zmax = thee->pmgp->zcent + (zlen/2.0);
04669
04670     /* This is a floating point parameter related to the non-zero nature of the
04671      * bulk ionic strength. If the ionic strength is greater than zero; this
04672      * parameter is set to 1.0 and later scaled by the appropriate pre-factors.
04673      * Otherwise, this parameter is set to 0.0 */
04674     if (ionstr > VPMGSMALL) ionmask = 1.0;
04675     else ionmask = 0.0;
04676
04677     /* Reset the kappa array, marking everything accessible */
04678     for (i=0; i<(nx*ny*nz); i++) thee->kappa[i] = ionmask;
04679
04680     if (ionstr < VPMGSMALL) return;
04681
04682     /* Loop through the atoms and set kappa = 0.0 (inaccessible) if a point
04683      * is inside the ion-inflated van der Waals radii */
04684     for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
04685
04686         atom = Valist_getAtom(alist, iatom);
04687         apos = Vatom_getPosition(atom);
04688         arad = Vatom_getRadius(atom);
04689
04690         if (arad > VSMALL) {
04691
04692

```

```

04693         /* Make sure we're on the grid */
04694         if ((apos[0]<(xmin-irad-arad)) || (apos[0]>(xmax+irad+arad)) || \
04695             (apos[1]<(ymin-irad-arad)) || (apos[1]>(ymax+irad+arad)) || \
04696             (apos[2]<(zmin-irad-arad)) || (apos[2]>(zmax+irad+arad))) {
04697             if ((thee->pmgp->bcfl != BCFL_FOCUS) &&
04698                 (thee->pmgp->bcfl != BCFL_MAP)) {
04699                 Vnm_print(2,
04700 "Vpmg_fillco: Atom #d at (%4.3f, %4.3f, %4.3f) is off the mesh (ignoring):\n",
04701                     iatom, apos[0], apos[1], apos[2]);
04702                 Vnm_print(2, "Vpmg_fillco:  xmin = %g, xmax = %g\n",
04703                     xmin, xmax);
04704                 Vnm_print(2, "Vpmg_fillco:  ymin = %g, ymax = %g\n",
04705                     ymin, ymax);
04706                 Vnm_print(2, "Vpmg_fillco:  zmin = %g, zmax = %g\n",
04707                     zmin, zmax);
04708             }
04709             fflush(stderr);
04710         } else { /* if we're on the mesh */
04711             /* Mark ions */
04712             markSphere((irad+arad), apos,
04713                 nx, ny, nz,
04714                 hx, hy, hzed,
04715                 xmin, ymin, zmin,
04716                 thee->kappa, 0.0);
04717         } /* endif (on the mesh) */
04718     }
04719 } /* endfor (over all atoms) */
04720 }
04721 }
04722 }
04723 }
04724 }
04725 }
04726 VPRIVATE void fillcoCoefMolDiel(Vpmg *thee) {
04727     /* Always call NoSmooth to fill the epsilon arrays */
04728     fillcoCoefMolDielNoSmooth(thee);
04729     /* Call the smoothing algorithm as needed */
04730     if (thee->surfMeth == VSM_MOLSMOOTH) {
04731         fillcoCoefMolDielSmooth(thee);
04732     }
04733 }
04734 }
04735 }
04736 }
04737 VPRIVATE void fillcoCoefMolDielNoSmooth(Vpmg *thee) {
04738     Vacci *acc;
04739     VacciSurf *asurf;
04740     Valist *alist;
04741     Vpbe *pbe;
04742     Vatom *atom;
04743     double xmin, xmax, ymin, ymax, zmin, zmax;
04744     double xlen, ylen, zlen, position[3];
04745     double srad, epsw, epsp, deps, area;
04746     double hx, hy, hzed, *apos, arad;
04747     int i, nx, ny, nz, ntot, iatom, ipt;
04748     /* Get PBE info */
04749     pbe = thee->pbe;
04750     acc = pbe->acc;
04751     alist = pbe->alist;
04752     srad = Vpbe_getSolventRadius(pbe);
04753     epsw = Vpbe_getSolventDiel(pbe);
04754     epsp = Vpbe_getSoluteDiel(pbe);
04755     /* Mesh info */
04756     nx = thee->pmgp->nx;
04757     ny = thee->pmgp->ny;
04758     nz = thee->pmgp->nz;
04759     hx = thee->pmgp->hx;
04760     hy = thee->pmgp->hy;
04761     hzed = thee->pmgp->hzed;
04762     /* Define the total domain size */
04763     xlen = thee->pmgp->xlen;
04764     ylen = thee->pmgp->ylen;
04765     zlen = thee->pmgp->zlen;
04766     /* Define the min/max dimensions */
04767     xmin = thee->pmgp->xcent - (xlen/2.0);
04768     ymin = thee->pmgp->ycent - (ylen/2.0);

```



```

04774     zmin = thee->pmgp->zcent - (zlen/2.0);
04775     xmax = thee->pmgp->xcent + (xlen/2.0);
04776     ymax = thee->pmgp->ycent + (ylen/2.0);
04777     zmax = thee->pmgp->zcent + (zlen/2.0);
04778
04779     /* Reset the arrays */
04780     ntot = nx*ny*nz;
04781     for (i=0; i<ntot; i++) {
04782         thee->epsx[i] = epsw;
04783         thee->epsy[i] = epsw;
04784         thee->epsz[i] = epsw;
04785     }
04786
04787     /* Loop through the atoms and set a{123}cf = 0.0 (inaccessible)
04788      * if a point is inside the solvent-inflated van der Waals radii */
04789 #pragma omp parallel for default(shared) private(iatom,atom,apos,arad)
04790     for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
04791
04792         atom = Valist_getAtom(alist, iatom);
04793         apos = Vatom_getPosition(atom);
04794         arad = Vatom_getRadius(atom);
04795
04796         /* Make sure we're on the grid */
04797         if ((apos[0]<=xmin) || (apos[0]>=xmax) || \
04798             (apos[1]<=ymin) || (apos[1]>=ymax) || \
04799             (apos[2]<=zmin) || (apos[2]>=zmax)) {
04800             if ((thee->pmgp->bcfl != BCFL_FOCUS) &&
04801                 (thee->pmgp->bcfl != BCFL_MAP)) {
04802                 Vnm_print(2, "Vpmg_fillco: Atom #%d at (%4.3f, %4.3f, \
04803 %4.3f) is off the mesh (ignoring):\n",
04804                     iatom, apos[0], apos[1], apos[2]);
04805                 Vnm_print(2, "Vpmg_fillco: xmin = %g, xmax = %g\n",
04806                     xmin, xmax);
04807                 Vnm_print(2, "Vpmg_fillco: ymin = %g, ymax = %g\n",
04808                     ymin, ymax);
04809                 Vnm_print(2, "Vpmg_fillco: zmin = %g, zmax = %g\n",
04810                     zmin, zmax);
04811             }
04812             fflush(stderr);
04813         } else { /* if we're on the mesh */
04814
04815             if (arad > VSMALL) {
04816                 /* Mark x-shifted dielectric */
04817                 markSphere((arad+srad), apos,
04818                     nx, ny, nz,
04819                     hx, hy, hzed,
04820                     (xmin+0.5*hx), ymin, zmin,
04821                     thee->epsx, epsp);
04822
04823                 /* Mark y-shifted dielectric */
04824                 markSphere((arad+srad), apos,
04825                     nx, ny, nz,
04826                     hx, hy, hzed,
04827                     xmin, (ymin+0.5*hy), zmin,
04828                     thee->epsy, epsp);
04829
04830                 /* Mark z-shifted dielectric */
04831                 markSphere((arad+srad), apos,
04832                     nx, ny, nz,
04833                     hx, hy, hzed,
04834                     xmin, ymin, (zmin+0.5*hzed),
04835                     thee->epsz, epsp);
04836             }
04837         }
04838     } /* endif (on the mesh) */
04839 } /* endfor (over all atoms) */
04840
04841 area = Vacc_SASA(acc, srad);
04842
04843 /* We only need to do the next step for non-zero solvent radii */
04844 if (srad > VSMALL) {
04845     /* Now loop over the solvent accessible surface points */
04846
04847 #pragma omp parallel for default(shared) private(iatom,atom,area,asurf,ipt,position)
04848     for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
04849         atom = Valist_getAtom(alist, iatom);
04850         area = Vacc_atomSASA(acc, srad, atom);
04851         if (area > 0.0 ) {
04852             asurf = Vacc_atomSASPoints(acc, srad, atom);
04853         }
04854     }

```

```

04855
04856      /* Use each point on the SAS to reset the solvent accessibility */
04857      /* TODO: Make sure we're not still wasting time here. */
04858      for (ipt=0; ipt<(asurf->npts); ipt++) {
04859
04860          position[0] = asurf->xpts[ipt];
04861          position[1] = asurf->ypts[ipt];
04862          position[2] = asurf->zpts[ipt];
04863
04864          /* Mark x-shifted dielectric */
04865          markSphere(srad, position,
04866                  nx, ny, nz,
04867                  hx, hy, hzed,
04868                  (xmin+0.5*hx), ymin, zmin,
04869                  thee->epsx, epsw);
04870
04871          /* Mark y-shifted dielectric */
04872          markSphere(srad, position,
04873                  nx, ny, nz,
04874                  hx, hy, hzed,
04875                  xmin, (ymin+0.5*hy), zmin,
04876                  thee->epsy, epsw);
04877
04878          /* Mark z-shifted dielectric */
04879          markSphere(srad, position,
04880                  nx, ny, nz,
04881                  hx, hy, hzed,
04882                  xmin, ymin, (zmin+0.5*hzed),
04883                  thee->epsz, epsw);
04884
04885      }
04886  }
04887 }
04888 }
04889 }
04890
04891 VPRIVATE void fillCoefMolDielSmooth(Vpmpg *thee) {
04892
04893     /* This function smoothes using a 9 point method based on
04894        Bruccoleri, et al. J Comput Chem 18 268-276 (1997). The nine points
04895        used are the shifted grid point and the 8 points that are 1/sqrt(2)
04896        grid spacings away. The harmonic mean of the 9 points is then used to
04897        find the overall dielectric value for the point in question. The use of
04898        this function assumes that the non-smoothed values were placed in the
04899        dielectric arrays by the fillCoefMolDielNoSmooth function.*/
04900
04901     Vpbe *pbe;
04902     double frac, epsw;
04903     int i, j, k, nx, ny, nz, numpts;
04904
04905     /* Mesh info */
04906     nx = thee->pmgpg->nx;
04907     ny = thee->pmgpg->ny;
04908     nz = thee->pmgpg->nz;
04909
04910     pbe = thee->pbe;
04911     epsw = Vpbe_getSolventDiel(pbe);
04912
04913     /* Copy the existing diel arrays to work arrays */
04914     for (i=0; i<(nx*ny*nz); i++) {
04915         thee->a1cf[i] = thee->epsx[i];
04916         thee->a2cf[i] = thee->epsy[i];
04917         thee->a3cf[i] = thee->epsz[i];
04918         thee->epsx[i] = epsw;
04919         thee->epsy[i] = epsw;
04920         thee->epsz[i] = epsw;
04921     }
04922
04923     /* Smooth the dielectric values */
04924     for (i=0; i<nx; i++) {
04925         for (j=0; j<ny; j++) {
04926             for (k=0; k<nz; k++) {
04927
04928                 /* Get the 8 points that are 1/sqrt(2) grid spacings away */
04929
04930                 /* Points for the X-shifted array */
04931                 frac = 1.0/thee->a1cf[IJK(i,j,k)];
04932                 frac += 1.0/thee->a2cf[IJK(i,j,k)];
04933                 frac += 1.0/thee->a3cf[IJK(i,j,k)];
04934                 numpts = 3;
04935

```

```

04936         if (j > 0) {
04937             frac += 1.0/thee->a2cf[IJK(i, j-1, k)];
04938             numpts += 1;
04939         }
04940         if (k > 0) {
04941             frac += 1.0/thee->a3cf[IJK(i, j, k-1)];
04942             numpts += 1;
04943         }
04944         if (i < (nx-1)){
04945             frac += 1.0/thee->a2cf[IJK(i+1, j, k)];
04946             frac += 1.0/thee->a3cf[IJK(i+1, j, k)];
04947             numpts += 2;
04948             if (j > 0) {
04949                 frac += 1.0/thee->a2cf[IJK(i+1, j-1, k)];
04950                 numpts += 1;
04951             }
04952             if (k > 0) {
04953                 frac += 1.0/thee->a3cf[IJK(i+1, j, k-1)];
04954                 numpts += 1;
04955             }
04956         }
04957         thee->epsx[IJK(i, j, k)] = numpts/frac;
04958
04959         /* Points for the Y-shifted array */
04960         frac = 1.0/thee->a2cf[IJK(i, j, k)];
04961         frac += 1.0/thee->a1cf[IJK(i, j, k)];
04962         frac += 1.0/thee->a3cf[IJK(i, j, k)];
04963         numpts = 3;
04964
04965         if (i > 0) {
04966             frac += 1.0/thee->a1cf[IJK(i-1, j, k)];
04967             numpts += 1;
04968         }
04969         if (k > 0) {
04970             frac += 1.0/thee->a3cf[IJK(i, j, k-1)];
04971             numpts += 1;
04972         }
04973         if (j < (ny-1)){
04974             frac += 1.0/thee->a1cf[IJK(i, j+1, k)];
04975             frac += 1.0/thee->a3cf[IJK(i, j+1, k)];
04976             numpts += 2;
04977             if (i > 0) {
04978                 frac += 1.0/thee->a1cf[IJK(i-1, j+1, k)];
04979                 numpts += 1;
04980             }
04981             if (k > 0) {
04982                 frac += 1.0/thee->a3cf[IJK(i, j+1, k-1)];
04983                 numpts += 1;
04984             }
04985         }
04986         thee->epsy[IJK(i, j, k)] = numpts/frac;
04987
04988         /* Points for the Z-shifted array */
04989         frac = 1.0/thee->a3cf[IJK(i, j, k)];
04990         frac += 1.0/thee->a1cf[IJK(i, j, k)];
04991         frac += 1.0/thee->a2cf[IJK(i, j, k)];
04992         numpts = 3;
04993
04994         if (i > 0) {
04995             frac += 1.0/thee->a1cf[IJK(i-1, j, k)];
04996             numpts += 1;
04997         }
04998         if (j > 0) {
04999             frac += 1.0/thee->a2cf[IJK(i, j-1, k)];
05000             numpts += 1;
05001         }
05002         if (k < (nz-1)){
05003             frac += 1.0/thee->a1cf[IJK(i, j, k+1)];
05004             frac += 1.0/thee->a2cf[IJK(i, j, k+1)];
05005             numpts += 2;
05006             if (i > 0) {
05007                 frac += 1.0/thee->a1cf[IJK(i-1, j, k+1)];
05008                 numpts += 1;
05009             }
05010             if (j > 0) {
05011                 frac += 1.0/thee->a2cf[IJK(i, j-1, k+1)];
05012                 numpts += 1;
05013             }
05014         }
05015         thee->epsz[IJK(i, j, k)] = numpts/frac;
05016     }

```

```

05017     }
05018     }
05019 }
05020
05021
05022 VPRIVATE void fillCoefSpline(Vpmg *thee) {
05023     Valist *alist;
05024     Vpbe *pbe;
05025     Vatom *atom;
05026     double xmin, xmax, ymin, ymax, zmin, zmax, ionmask, ionstr, dist2;
05027     double xlen, ylen, zlen, position[3], itot, stot, ictot, ictot2, sctot;
05028     double irad, dx, dy, dz, epsw, epsp, w2i;
05029     double hx, hy, hzed, *apos, arad, sctot2;
05030     double dx2, dy2, dz2, stot2, itot2, rtot, rtot2, splineWin, w3i;
05031     double dist, value, sm, sm2;
05032     int i, j, k, nx, ny, nz, iatom;
05033     int imin, imax, jmin, jmax, kmin, kmax;
05034
05035     VASSERT(thee != VNULL);
05036     splineWin = thee->splineWin;
05037     w2i = 1.0/(splineWin*splineWin);
05038     w3i = 1.0/(splineWin*splineWin*splineWin);
05039
05040     /* Get PBE info */
05041     pbe = thee->pbe;
05042     alist = pbe->alist;
05043     irad = Vpbe_getMaxIonRadius(pbe);
05044     ionstr = Vpbe_getBulkIonicStrength(pbe);
05045     epsw = Vpbe_getSolventDiel(pbe);
05046     epsp = Vpbe_getSoluteDiel(pbe);
05047
05048     /* Mesh info */
05049     nx = thee->pmgp->nx;
05050     ny = thee->pmgp->ny;
05051     nz = thee->pmgp->nz;
05052     hx = thee->pmgp->hx;
05053     hy = thee->pmgp->hy;
05054     hzed = thee->pmgp->hzed;
05055
05056     /* Define the total domain size */
05057     xlen = thee->pmgp->xlen;
05058     ylen = thee->pmgp->ylen;
05059     zlen = thee->pmgp->zlen;
05060
05061     /* Define the min/max dimensions */
05062     xmin = thee->pmgp->xcent - (xlen/2.0);
05063     ymin = thee->pmgp->ycent - (ylen/2.0);
05064     zmin = thee->pmgp->zcent - (zlen/2.0);
05065     xmax = thee->pmgp->xcent + (xlen/2.0);
05066     ymax = thee->pmgp->ycent + (ylen/2.0);
05067     zmax = thee->pmgp->zcent + (zlen/2.0);
05068
05069     /* This is a floating point parameter related to the non-zero nature of the
05070      * bulk ionic strength. If the ionic strength is greater than zero; this
05071      * parameter is set to 1.0 and later scaled by the appropriate pre-factors.
05072      * Otherwise, this parameter is set to 0.0 */
05073     if (ionstr > VPMGSMALL) ionmask = 1.0;
05074     else ionmask = 0.0;
05075
05076     /* Reset the kappa, epsx, epsy, and epsz arrays */
05077     for (i=0; i<(nx*ny*nz); i++) {
05078         thee->kappa[i] = 1.0;
05079         thee->epsx[i] = 1.0;
05080         thee->epsy[i] = 1.0;
05081         thee->epsz[i] = 1.0;
05082     }
05083
05084     /* Loop through the atoms and do assign the dielectric */
05085     for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
05086         atom = Valist_getAtom(alist, iatom);
05087         apos = Vatom_getPosition(atom);
05088         arad = Vatom_getRadius(atom);
05089
05090         /* Make sure we're on the grid */
05091         if ((apos[0]<=xmin) || (apos[0]>=xmax) || \
05092             (apos[1]<=ymin) || (apos[1]>=ymax) || \
05093             (apos[2]<=zmin) || (apos[2]>=zmax)) {
05094             if ((thee->pmgp->bcfl != BCFL_FOCUS) &&
05095                 (thee->pmgp->bcfl != BCFL_MAP)) {

```

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05098         Vnm_print(2, "Vpmg_fillco: Atom #d at (%4.3f, %4.3f,\
05099 %4.3f) is off the mesh (ignoring):\n",
05100         iatom, apos[0], apos[1], apos[2]);
05101         Vnm_print(2, "Vpmg_fillco: xmin = %g, xmax = %g\n",
05102         xmin, xmax);
05103         Vnm_print(2, "Vpmg_fillco: ymin = %g, ymax = %g\n",
05104         ymin, ymax);
05105         Vnm_print(2, "Vpmg_fillco: zmin = %g, zmax = %g\n",
05106         zmin, zmax);
05107     }
05108     fflush(stderr);
05109
05110     } else if (arad > VPMGSMALL) { /* if we're on the mesh */
05111
05112         /* Convert the atom position to grid reference frame */
05113         position[0] = apos[0] - xmin;
05114         position[1] = apos[1] - ymin;
05115         position[2] = apos[2] - zmin;
05116
05117         /* MARK ION ACCESSIBILITY AND DIELECTRIC VALUES FOR LATER
05118          * ASSIGNMENT (Steps #1-3) */
05119         itot = irad + arad + splineWin;
05120         itot2 = VSQR(itot);
05121         ictot = VMAX2(0, (irad + arad - splineWin));
05122         ictot2 = VSQR(ictot);
05123         stot = arad + splineWin;
05124         stot2 = VSQR(stot);
05125         sctot = VMAX2(0, (arad - splineWin));
05126         sctot2 = VSQR(sctot);
05127
05128         /* We'll search over grid points which are in the greater of
05129          * these two radii */
05130         rtot = VMAX2(itot, stot);
05131         rtot2 = VMAX2(itot2, stot2);
05132         dx = rtot + 0.5*hx;
05133         dy = rtot + 0.5*hy;
05134         dz = rtot + 0.5*hzed;
05135         imin = VMAX2(0, (int)floor((position[0] - dx)/hx));
05136         imax = VMIN2(nx-1, (int)ceil((position[0] + dx)/hx));
05137         jmin = VMAX2(0, (int)floor((position[1] - dy)/hy));
05138         jmax = VMIN2(ny-1, (int)ceil((position[1] + dy)/hy));
05139         kmin = VMAX2(0, (int)floor((position[2] - dz)/hzed));
05140         kmax = VMIN2(nz-1, (int)ceil((position[2] + dz)/hzed));
05141         for (i=imin; i<=imax; i++) {
05142             dx2 = VSQR(position[0] - hx*i);
05143             for (j=jmin; j<=jmax; j++) {
05144                 dy2 = VSQR(position[1] - hy*j);
05145                 for (k=kmin; k<=kmax; k++) {
05146                     dz2 = VSQR(position[2] - k*hzed);
05147
05148                     /* ASSIGN CCF */
05149                     if (thee->kappa[IJK(i,j,k)] > VPMGSMALL) {
05150                         dist2 = dz2 + dy2 + dx2;
05151                         if (dist2 >= itot2) {
05152                             ;
05153                         }
05154                         if (dist2 <= ictot2) {
05155                             thee->kappa[IJK(i,j,k)] = 0.0;
05156                         }
05157                         if ((dist2 < itot2) && (dist2 > ictot2)) {
05158                             dist = VSQRT(dist2);
05159                             sm = dist - (arad + irad) + splineWin;
05160                             sm2 = VSQR(sm);
05161                             value = 0.75*sm2*w2i - 0.25*sm*sm2*w3i;
05162                             thee->kappa[IJK(i,j,k)] *= value;
05163                         }
05164                     }
05165
05166                     /* ASSIGN A1CF */
05167                     if (thee->epsx[IJK(i,j,k)] > VPMGSMALL) {
05168                         dist2 = dz2+dy2+VSQR(position[0]-(i+0.5)*hx);
05169                         if (dist2 >= stot2) {
05170                             thee->epsx[IJK(i,j,k)] *= 1.0;
05171                         }
05172                         if (dist2 <= sctot2) {
05173                             thee->epsx[IJK(i,j,k)] = 0.0;
05174                         }
05175                         if ((dist2 > sctot2) && (dist2 < stot2)) {
05176                             dist = VSQRT(dist2);
05177                             sm = dist - arad + splineWin;
05178                             sm2 = VSQR(sm);

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05179         value = 0.75*sm2*w2i - 0.25*sm*sm2*w3i;
05180         thee->epsx[IJK(i,j,k)] *= value;
05181     }
05182 }
05183
05184 /* ASSIGN A2CF */
05185 if (thee->epsy[IJK(i,j,k)] > VPMGSMALL) {
05186     dist2 = dz2+dx2+VSQR(position[1]-(j+0.5)*hy);
05187     if (dist2 >= stot2) {
05188         thee->epsy[IJK(i,j,k)] *= 1.0;
05189     }
05190     if (dist2 <= sctot2) {
05191         thee->epsy[IJK(i,j,k)] = 0.0;
05192     }
05193     if ((dist2 > sctot2) && (dist2 < stot2)) {
05194         dist = VSQRT(dist2);
05195         sm = dist - arad + splineWin;
05196         sm2 = VSQR(sm);
05197         value = 0.75*sm2*w2i - 0.25*sm*sm2*w3i;
05198         thee->epsy[IJK(i,j,k)] *= value;
05199     }
05200 }
05201
05202 /* ASSIGN A3CF */
05203 if (thee->epsz[IJK(i,j,k)] > VPMGSMALL) {
05204     dist2 = dy2+dx2+VSQR(position[2]-(k+0.5)*hzed);
05205     if (dist2 >= stot2) {
05206         thee->epsz[IJK(i,j,k)] *= 1.0;
05207     }
05208     if (dist2 <= sctot2) {
05209         thee->epsz[IJK(i,j,k)] = 0.0;
05210     }
05211     if ((dist2 > sctot2) && (dist2 < stot2)) {
05212         dist = VSQRT(dist2);
05213         sm = dist - arad + splineWin;
05214         sm2 = VSQR(sm);
05215         value = 0.75*sm2*w2i - 0.25*sm*sm2*w3i;
05216         thee->epsz[IJK(i,j,k)] *= value;
05217     }
05218 }
05219
05220
05221     } /* k loop */
05222 } /* j loop */
05223 } /* i loop */
05224 } /* endif (on the mesh) */
05225 } /* endfor (over all atoms) */
05226
05227 Vnm_print(0, "Vpmg_fillco: filling coefficient arrays\n");
05228 /* Interpret markings and fill the coefficient arrays */
05229 for (k=0; k<nz; k++) {
05230     for (j=0; j<ny; j++) {
05231         for (i=0; i<nx; i++) {
05232
05233             thee->kappa[IJK(i,j,k)] = ionmask*thee->kappa[IJK(i,j,k)];
05234             thee->epsx[IJK(i,j,k)] = (epsw-epsp)*thee->epsx[IJK(i,j,k)]
05235                 + epsp;
05236             thee->epsy[IJK(i,j,k)] = (epsw-epsp)*thee->epsy[IJK(i,j,k)]
05237                 + epsp;
05238             thee->epsz[IJK(i,j,k)] = (epsw-epsp)*thee->epsz[IJK(i,j,k)]
05239                 + epsp;
05240
05241         } /* i loop */
05242     } /* j loop */
05243 } /* k loop */
05244
05245 }
05246
05247 VPRIVATE void fillcoCoef(Vpmg *thee) {
05248     VASSERT(thee != VNULL);
05249
05250     if (thee->useDielXMap || thee->useDielYMap ||
05251         thee->useDielZMap || thee->useKappaMap) {
05252         fillcoCoefMap(thee);
05253         return;
05254     }
05255
05256     switch(thee->surfMeth) {
05257     case VSM_MOL:
05258         Vnm_print(0, "fillcoCoef: Calling fillcoCoefMol...\n");

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```

05260         fillcoCoefMol(thee);
05261         break;
05262     case VSM_MOLSMOOTH:
05263         Vnm_print(0, "fillcoCoef: Calling fillcoCoefMol...\n");
05264         fillcoCoefMol(thee);
05265         break;
05266     case VSM_SPLINE:
05267         Vnm_print(0, "fillcoCoef: Calling fillcoCoefSpline...\n");
05268         fillcoCoefSpline(thee);
05269         break;
05270     case VSM_SPLINE3:
05271         Vnm_print(0, "fillcoCoef: Calling fillcoCoefSpline3...\n");
05272         fillcoCoefSpline3(thee);
05273         break;
05274     case VSM_SPLINE4:
05275         Vnm_print(0, "fillcoCoef: Calling fillcoCoefSpline4...\n");
05276         fillcoCoefSpline4(thee);
05277         break;
05278     default:
05279         Vnm_print(2, "fillcoCoef: Invalid surfMeth (%d)!\n",
05280                 thee->surfMeth);
05281         VASSERT(0);
05282         break;
05283     }
05284 }
05285
05286
05287 VPRIVATE Vrc_Codes fillcoCharge(Vpmg *thee) {
05288     Vrc_Codes rc;
05289
05290     VASSERT(thee != VNULL);
05291
05292     if (thee->useChargeMap) {
05293         return fillcoChargeMap(thee);
05294     }
05295
05296     switch(thee->chargeMeth) {
05297     case VCM_TRIL:
05298         Vnm_print(0, "fillcoCharge: Calling fillcoChargeSpline1...\n");
05299         fillcoChargeSpline1(thee);
05300         break;
05301     case VCM_BSPL2:
05302         Vnm_print(0, "fillcoCharge: Calling fillcoChargeSpline2...\n");
05303         fillcoChargeSpline2(thee);
05304         break;
05305     case VCM_BSPL4:
05306         switch (thee->chargeSrc) {
05307         case VCM_CHARGE:
05308             Vnm_print(0, "fillcoCharge: Calling fillcoPermanentMultipole...\n");
05309             fillcoPermanentMultipole(thee);
05310             break;
05311         #if defined(WITH_TINKER)
05312         case VCM_PERMANENT:
05313             Vnm_print(0, "fillcoCharge: Calling fillcoPermanentMultipole...\n");
05314             fillcoPermanentMultipole(thee);
05315             break;
05316         case VCM_INDUCED:
05317             Vnm_print(0, "fillcoCharge: Calling fillcoInducedDipole...\n");
05318             fillcoInducedDipole(thee);
05319             break;
05320         case VCM_NLINDUCED:
05321             Vnm_print(0, "fillcoCharge: Calling fillcoNLInducedDipole...\n");
05322             fillcoNLInducedDipole(thee);
05323             break;
05324         #endif /* if defined(WITH_TINKER) */
05325         default:
05326             Vnm_print(2, "fillcoCharge: Invalid chargeSource (%d)!\n",
05327                     thee->chargeSrc);
05328             return VRC_FAILURE;
05329             break;
05330         }
05331     }
05332     break;
05333     default:
05334         Vnm_print(2, "fillcoCharge: Invalid chargeMeth (%d)!\n",
05335                 thee->chargeMeth);
05336         return VRC_FAILURE;
05337         break;
05338     }
05339
05340     return VRC_SUCCESS;

```

```

05341 }
05342
05343 VPRIVATE Vrc_Codes fillcoChargeMap(Vpmg *thee) {
05344
05345     Vpbe *pbe;
05346     double position[3], charge, zmagic, hx, hy, hzed;
05347     int i, j, k, nx, ny, nz, rc;
05348
05349
05350     VASSERT(thee != VNULL);
05351
05352     /* Get PBE info */
05353     pbe = thee->pbe;
05354     zmagic = Vpbe_getZmagic(pbe);
05355
05356     /* Mesh info */
05357     nx = thee->pmgp->nx;
05358     ny = thee->pmgp->ny;
05359     nz = thee->pmgp->nz;
05360     hx = thee->pmgp->hx;
05361     hy = thee->pmgp->hy;
05362     hzed = thee->pmgp->hzed;
05363
05364     /* Reset the charge array */
05365     for (i=0; i<(nx*ny*nz); i++) thee->charge[i] = 0.0;
05366
05367     /* Fill in the source term (atomic charges) */
05368     Vnm_print(0, "Vpmg_fillco: filling in source term.\n");
05369     for (k=0; k<nz; k++) {
05370         for (j=0; j<ny; j++) {
05371             for (i=0; i<nx; i++) {
05372                 position[0] = thee->xf[i];
05373                 position[1] = thee->yf[j];
05374                 position[2] = thee->zf[k];
05375                 rc = Vgrid_value(thee->chargeMap, position, &charge);
05376                 if (!rc) {
05377                     Vnm_print(2, "fillcoChargeMap: Error -- fell off of charge map at (%g, %g, %g)!\n",
05378                             position[0], position[1], position[2]);
05379                     return VRC_FAILURE;
05380                 }
05381                 /* Scale the charge to internal units */
05382                 charge = charge*zmagic;
05383                 thee->charge[IJK(i,j,k)] = charge;
05384             }
05385         }
05386     }
05387
05388     return VRC_SUCCESS;
05389 }
05390
05391 VPRIVATE void fillcoChargesSpline1(Vpmg *thee) {
05392
05393     Valist *alist;
05394     Vpbe *pbe;
05395     Vatom *atom;
05396     double xmin, xmax, ymin, ymax, zmin, zmax;
05397     double xlen, ylen, zlen, position[3], ifloat, jfloat, kfloat;
05398     double charge, dx, dy, dz, zmagic, hx, hy, hzed, *apos;
05399     int i, nx, ny, nz, iatom, ihi, ilo, jhi, jlo, khi, klo;
05400
05401
05402     VASSERT(thee != VNULL);
05403
05404     /* Get PBE info */
05405     pbe = thee->pbe;
05406     alist = pbe->alist;
05407     zmagic = Vpbe_getZmagic(pbe);
05408
05409     /* Mesh info */
05410     nx = thee->pmgp->nx;
05411     ny = thee->pmgp->ny;
05412     nz = thee->pmgp->nz;
05413     hx = thee->pmgp->hx;
05414     hy = thee->pmgp->hy;
05415     hzed = thee->pmgp->hzed;
05416
05417     /* Define the total domain size */
05418     xlen = thee->pmgp->xlen;
05419     ylen = thee->pmgp->ylen;
05420     zlen = thee->pmgp->zlen;
05421

```



```

05422      /* Define the min/max dimensions */
05423      xmin = thee->pmgp->xcent - (xlen/2.0);
05424      ymin = thee->pmgp->ycent - (ylen/2.0);
05425      zmin = thee->pmgp->zcent - (zlen/2.0);
05426      xmax = thee->pmgp->xcent + (xlen/2.0);
05427      ymax = thee->pmgp->ycent + (ylen/2.0);
05428      zmax = thee->pmgp->zcent + (zlen/2.0);
05429
05430      /* Reset the charge array */
05431      for (i=0; i<(nx*ny*nz); i++) thee->charge[i] = 0.0;
05432
05433      /* Fill in the source term (atomic charges) */
05434      Vnm_print(0, "Vpmg_fillco: filling in source term.\n");
05435      for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
05436
05437          atom = Valist_getAtom(alist, iatom);
05438          apos = Vatom_getPosition(atom);
05439          charge = Vatom_getCharge(atom);
05440
05441          /* Make sure we're on the grid */
05442          if ((apos[0]<=xmin) || (apos[0]>=xmax) || \
05443              (apos[1]<=ymin) || (apos[1]>=ymax) || \
05444              (apos[2]<=zmin) || (apos[2]>=zmax)) {
05445              if ((thee->pmgp->bcfl != BCFL_FOCUS) &&
05446                  (thee->pmgp->bcfl != BCFL_MAP)) {
05447                  Vnm_print(2, "Vpmg_fillco: Atom #%d at (%4.3f, %4.3f, \
05448 %4.3f) is off the mesh (ignoring):\n",
05449                      iatom, apos[0], apos[1], apos[2]);
05450                  Vnm_print(2, "Vpmg_fillco:      xmin = %g, xmax = %g\n",
05451                      xmin, xmax);
05452                  Vnm_print(2, "Vpmg_fillco:      ymin = %g, ymax = %g\n",
05453                      ymin, ymax);
05454                  Vnm_print(2, "Vpmg_fillco:      zmin = %g, zmax = %g\n",
05455                      zmin, zmax);
05456              }
05457              fflush(stderr);
05458          } else {
05459
05460              /* Convert the atom position to grid reference frame */
05461              position[0] = apos[0] - xmin;
05462              position[1] = apos[1] - ymin;
05463              position[2] = apos[2] - zmin;
05464
05465              /* Scale the charge to be a delta function */
05466              charge = charge*zmagic/(hx*hy*hzed);
05467
05468              /* Figure out which vertices we're next to */
05469              ifloat = position[0]/hx;
05470              jfloat = position[1]/hy;
05471              kfloat = position[2]/hzed;
05472
05473              ihi = (int)ceil(ifloat);
05474              ilo = (int)floor(ifloat);
05475              jhi = (int)ceil(jfloat);
05476              jlo = (int)floor(jfloat);
05477              khi = (int)ceil(kfloat);
05478              klo = (int)floor(kfloat);
05479
05480              /* Now assign fractions of the charge to the nearby verts */
05481              dx = ifloat - (double)(ilo);
05482              dy = jfloat - (double)(jlo);
05483              dz = kfloat - (double)(klo);
05484              thee->charge[IJK(ihi, jhi, khi)] += (dx*dy*dz*charge);
05485              thee->charge[IJK(ihi, jlo, khi)] += (dx*(1.0-dy)*dz*charge);
05486              thee->charge[IJK(ihi, jhi, klo)] += (dx*dy*(1.0-dz)*charge);
05487              thee->charge[IJK(ihi, jlo, klo)] += (dx*(1.0-dy)*(1.0-dz)*charge);
05488              thee->charge[IJK(ilo, jhi, khi)] += ((1.0-dx)*dy*dz *charge);
05489              thee->charge[IJK(ilo, jlo, khi)] += ((1.0-dx)*(1.0-dy)*dz *charge);
05490              thee->charge[IJK(ilo, jhi, klo)] += ((1.0-dx)*dy*(1.0-dz)*charge);
05491              thee->charge[IJK(ilo, jlo, klo)] += ((1.0-dx)*(1.0-dy)*(1.0-dz)*charge);
05492          } /* endif (on the mesh) */
05493      } /* endfor (each atom) */
05494  }
05495
05496  VPRIVATE double bspline2(double x) {
05497
05498      double m2m, m2, m3;
05499
05500      if ((x >= 0.0) && (x <= 2.0)) m2m = 1.0 - VABS(x - 1.0);
05501      else m2m = 0.0;
05502      if ((x >= 1.0) && (x <= 3.0)) m2 = 1.0 - VABS(x - 2.0);

```

```

05503     else m2 = 0.0;
05504
05505     if ((x >= 0.0) && (x <= 3.0)) m3 = 0.5*x*m2m + 0.5*(3.0-x)*m2;
05506     else m3 = 0.0;
05507
05508     return m3;
05509 }
05510
05511
05512 VPRIVATE double dbspline2(double x) {
05513
05514     double m2m, m2, dm3;
05515
05516     if ((x >= 0.0) && (x <= 2.0)) m2m = 1.0 - VABS(x - 1.0);
05517     else m2m = 0.0;
05518     if ((x >= 1.0) && (x <= 3.0)) m2 = 1.0 - VABS(x - 2.0);
05519     else m2 = 0.0;
05520
05521     dm3 = m2m - m2;
05522
05523     return dm3;
05524 }
05525
05526
05527
05528 VPRIVATE void fillcoChargeSpline2(Vpmg *thee) {
05529
05530     Valist *alist;
05531     Vpbe *pbe;
05532     Vatom *atom;
05533     double xmin, xmax, ymin, ymax, zmin, zmax, zmagic;
05534     double xlen, ylen, zlen, position[3], ifloat, jfloat, kfloat;
05535     double charge, hx, hy, hzed, *apos, mx, my, mz;
05536     int i, ii, jj, kk, nx, ny, nz, iatom;
05537     int im2, im1, ip1, ip2, jm2, jm1, jp1, jp2, km2, km1, kp1, kp2;
05538
05539
05540     VASSERT(thee != VNULL);
05541
05542     /* Get PBE info */
05543     pbe = thee->pbe;
05544     alist = pbe->alist;
05545     zmagic = Vpbe_getZmagic(pbe);
05546
05547     /* Mesh info */
05548     nx = thee->pmgp->nx;
05549     ny = thee->pmgp->ny;
05550     nz = thee->pmgp->nz;
05551     hx = thee->pmgp->hx;
05552     hy = thee->pmgp->hy;
05553     hzed = thee->pmgp->hzed;
05554
05555     /* Define the total domain size */
05556     xlen = thee->pmgp->xlen;
05557     ylen = thee->pmgp->ylen;
05558     zlen = thee->pmgp->zlen;
05559
05560     /* Define the min/max dimensions */
05561     xmin = thee->pmgp->xcent - (xlen/2.0);
05562     ymin = thee->pmgp->ycent - (ylen/2.0);
05563     zmin = thee->pmgp->zcent - (zlen/2.0);
05564     xmax = thee->pmgp->xcent + (xlen/2.0);
05565     ymax = thee->pmgp->ycent + (ylen/2.0);
05566     zmax = thee->pmgp->zcent + (zlen/2.0);
05567
05568     /* Reset the charge array */
05569     for (i=0; i<(nx*ny*nz); i++) thee->charge[i] = 0.0;
05570
05571     /* Fill in the source term (atomic charges) */
05572     Vnm_print(0, "Vpmg_fillco: filling in source term.\n");
05573     for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
05574
05575         atom = Valist_getAtom(alist, iatom);
05576         apos = Vatom_getPosition(atom);
05577         charge = Vatom_getCharge(atom);
05578
05579         /* Make sure we're on the grid */
05580         if ((apos[0]<=(xmin-hx)) || (apos[0]>=(xmax+hx)) || \
05581             (apos[1]<=(ymin-hy)) || (apos[1]>=(ymax+hy)) || \
05582             (apos[2]<=(zmin-hzed)) || (apos[2]>=(zmax+hzed))) {
05583             if ((thee->pmgp->bcfl != BCFL_FOCUS) &&

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05584         (thee->pmgp->bcfl != BCFL_MAP)) {
05585             Vnm_print(2, "Vpmg_fillco: Atom #%d at (%4.3f, %4.3f, \
05586 %4.3f) is off the mesh (for cubic splines!!) (ignoring this atom):\n",
05587                     iatom, apos[0], apos[1], apos[2]);
05588             Vnm_print(2, "Vpmg_fillco:      xmin = %g, xmax = %g\n",
05589                     xmin, xmax);
05590             Vnm_print(2, "Vpmg_fillco:      ymin = %g, ymax = %g\n",
05591                     ymin, ymax);
05592             Vnm_print(2, "Vpmg_fillco:      zmin = %g, zmax = %g\n",
05593                     zmin, zmax);
05594         }
05595         fflush(stderr);
05596     } else {
05597
05598         /* Convert the atom position to grid reference frame */
05599         position[0] = apos[0] - xmin;
05600         position[1] = apos[1] - ymin;
05601         position[2] = apos[2] - zmin;
05602
05603         /* Scale the charge to be a delta function */
05604         charge = charge*zmagic/(hx*hy*hzed);
05605
05606         /* Figure out which vertices we're next to */
05607         ifloat = position[0]/hx;
05608         jfloat = position[1]/hy;
05609         kfloat = position[2]/hzed;
05610
05611         ip1 = (int)ceil(ifloat);
05612         ip2 = ip1 + 1;
05613         im1 = (int)floor(ifloat);
05614         im2 = im1 - 1;
05615         jp1 = (int)ceil(jfloat);
05616         jp2 = jp1 + 1;
05617         jm1 = (int)floor(jfloat);
05618         jm2 = jm1 - 1;
05619         kp1 = (int)ceil(kfloat);
05620         kp2 = kp1 + 1;
05621         km1 = (int)floor(kfloat);
05622         km2 = km1 - 1;
05623
05624         /* This step shouldn't be necessary, but it saves nasty debugging
05625          * later on if something goes wrong */
05626         ip2 = VMIN2(ip2, nx-1);
05627         ip1 = VMIN2(ip1, nx-1);
05628         im1 = VMAX2(im1, 0);
05629         im2 = VMAX2(im2, 0);
05630         jp2 = VMIN2(jp2, ny-1);
05631         jp1 = VMIN2(jp1, ny-1);
05632         jm1 = VMAX2(jm1, 0);
05633         jm2 = VMAX2(jm2, 0);
05634         kp2 = VMIN2(kp2, nz-1);
05635         kp1 = VMIN2(kp1, nz-1);
05636         km1 = VMAX2(km1, 0);
05637         km2 = VMAX2(km2, 0);
05638
05639         /* Now assign fractions of the charge to the nearby verts */
05640         for (ii=im2; ii<=ip2; ii++) {
05641             mx = bspline2(VFCHI(ii, ifloat));
05642             for (jj=jm2; jj<=jp2; jj++) {
05643                 my = bspline2(VFCHI(jj, jfloat));
05644                 for (kk=km2; kk<=kp2; kk++) {
05645                     mz = bspline2(VFCHI(kk, kfloat));
05646                     thee->charge[IJK(ii, jj, kk)] += (charge*mx*my*mz);
05647                 }
05648             }
05649         }
05650
05651     } /* endif (on the mesh) */
05652 } /* endfor (each atom) */
05653 }
05654
05655 VPUBLIC int Vpmg_fillco(Vpmg *thee,
05656                        Vsurf_Meth surfMeth,
05657                        double splineWin,
05658                        Vchrg_Meth chargeMeth,
05659                        int useDielXMap,
05660                        Vgrid *dielXMap,
05661                        int useDielYMap,
05662                        Vgrid *dielYMap,
05663                        int useDielZMap,
05664                        Vgrid *dielZMap,

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05665             int useKappaMap,
05666             Vgrid *kappaMap,
05667             int usePotMap,
05668             Vgrid *potMap,
05669             int useChargeMap,
05670             Vgrid *chargeMap
05671         ) {
05672
05673         Vpbe *pbe;
05674         double xmin,
05675             xmax,
05676             ymin,
05677             ymax,
05678             zmin,
05679             zmax,
05680             xlen,
05681             ylen,
05682             zlen,
05683             hx,
05684             hy,
05685             hzed,
05686             epsw,
05687             epsp,
05688             ionstr;
05689         int i,
05690             nx,
05691             ny,
05692             nz,
05693             islap;
05694         Vrc_Codes rc;
05695
05696         if (thee == VNULL) {
05697             Vnm_print(2, "Vpmg_fillco: got NULL thee!\n");
05698             return 0;
05699         }
05700
05701         thee->surfMeth = surfMeth;
05702         thee->splineWin = splineWin;
05703         thee->chargeMeth = chargeMeth;
05704         thee->useDielXMap = useDielXMap;
05705         if (thee->useDielXMap) thee->dielXMap = dielXMap;
05706         thee->useDielYMap = useDielYMap;
05707         if (thee->useDielYMap) thee->dielYMap = dielYMap;
05708         thee->useDielZMap = useDielZMap;
05709         if (thee->useDielZMap) thee->dielZMap = dielZMap;
05710         thee->useKappaMap = useKappaMap;
05711         if (thee->useKappaMap) thee->kappaMap = kappaMap;
05712         thee->usePotMap = usePotMap;
05713         if (thee->usePotMap) thee->potMap = potMap;
05714         thee->useChargeMap = useChargeMap;
05715         if (thee->useChargeMap) thee->chargeMap = chargeMap;
05716
05717         /* Get PBE info */
05718         pbe = thee->pbe;
05719         ionstr = Vpbe_getBulkIonicStrength(pbe);
05720         epsw = Vpbe_getSolventDiel(pbe);
05721         epsp = Vpbe_getSoluteDiel(pbe);
05722
05723         /* Mesh info */
05724         nx = thee->pmgp->nx;
05725         ny = thee->pmgp->ny;
05726         nz = thee->pmgp->nz;
05727         hx = thee->pmgp->hx;
05728         hy = thee->pmgp->hy;
05729         hzed = thee->pmgp->hzed;
05730
05731         /* Define the total domain size */
05732         xlen = thee->pmgp->xlen;
05733         ylen = thee->pmgp->ylen;
05734         zlen = thee->pmgp->zlen;
05735
05736         /* Define the min/max dimensions */
05737         xmin = thee->pmgp->xcent - (xlen/2.0);
05738         thee->pmgp->xmin = xmin;
05739         ymin = thee->pmgp->ycent - (ylen/2.0);
05740         thee->pmgp->ymin = ymin;
05741         zmin = thee->pmgp->zcent - (zlen/2.0);
05742         thee->pmgp->zmin = zmin;
05743         xmax = thee->pmgp->xcent + (xlen/2.0);
05744         thee->pmgp->xmax = xmax;
05745         ymax = thee->pmgp->ycent + (ylen/2.0);

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05746     thee->pmgp->yymax = ymax;
05747     zmax = thee->pmgp->zcent + (zlen/2.0);
05748     thee->pmgp->zmax = zmax;
05749     thee->rparm[2] = xmin;
05750     thee->rparm[3] = xmax;
05751     thee->rparm[4] = ymin;
05752     thee->rparm[5] = ymax;
05753     thee->rparm[6] = zmin;
05754     thee->rparm[7] = zmax;
05755
05756     /* This is a flag that gets set if the operator is a simple Laplacian;
05757      * i.e., in the case of a homogenous dielectric and zero ionic strength
05758      * The operator cannot be a simple Laplacian if maps are read in. */
05759     if (thee->useDiexMap || thee->useDielyMap || thee->useDieltZMap ||
05760         thee->useKappaMap || thee->usePotMap) {
05761         islap = 0;
05762     } else if ( (ionstr < VPMGSMALL) && (VABS(epsp-epsw) < VPMGSMALL) ) {
05763         islap = 1;
05764     } else {
05765         islap = 0;
05766     }
05767
05768     /* Fill the mesh point coordinate arrays */
05769     for (i=0; i<nx; i++) thee->xf[i] = xmin + i*hx;
05770     for (i=0; i<ny; i++) thee->yf[i] = ymin + i*hy;
05771     for (i=0; i<nz; i++) thee->zf[i] = zmin + i*hzed;
05772
05773     /* Reset the tcf array */
05774     for (i=0; i<(nx*ny*nz); i++) thee->tcf[i] = 0.0;
05775
05776     /* Fill in the source term (atomic charges) */
05777     Vnm_print(0, "Vpmg_fillco: filling in source term.\n");
05778     rc = fillcoCharge(thee);
05779     switch(rc) {
05780         case VRC_SUCCESS:
05781             break;
05782         case VRC_WARNING:
05783             Vnm_print(2, "Vpmg_fillco: non-fatal errors while filling charge map!\n");
05784             break;
05785         case VRC_FAILURE:
05786             Vnm_print(2, "Vpmg_fillco: fatal errors while filling charge map!\n");
05787             return 0;
05788             break;
05789     }
05790
05791     /* THE FOLLOWING NEEDS TO BE DONE IF WE'RE NOT USING A SIMPLE LAPLACIAN
05792      * OPERATOR */
05793     if (!islap) {
05794         Vnm_print(0, "Vpmg_fillco: marking ion and solvent accessibility.\n");
05795         fillcoCoef(thee);
05796         Vnm_print(0, "Vpmg_fillco: done filling coefficient arrays\n");
05797     } else { /* else (!islap) ==> It's a Laplacian operator! */
05798
05799         for (i=0; i<(nx*ny*nz); i++) {
05800             thee->kappa[i] = 0.0;
05801             thee->epsx[i] = epsp;
05802             thee->epsy[i] = epsp;
05803             thee->epsz[i] = epsp;
05804         }
05805     }
05806
05807     } /* endif (!islap) */
05808
05809     /* Fill the boundary arrays (except when focusing, bcfl = 4) */
05810     if (thee->pmgp->bcfl != BCFL_FOCUS) {
05811         Vnm_print(0, "Vpmg_fillco: filling boundary arrays\n");
05812         bcCalc(thee);
05813         Vnm_print(0, "Vpmg_fillco: done filling boundary arrays\n");
05814     }
05815
05816     thee->filled = 1;
05817
05818     return 1;
05819 }
05820
05821
05822 VPUBLIC int Vpmg_force(Vpmg *thee, double *force, int atomID,
05823     Vsurf_Meth srfm, Vchrg_Meth chgm) {
05824
05825     int rc = 1;
05826     double qfF[3]; /* Charge-field force */

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```

05827     double dbF[3];                /* Dielectric boundary force */
05828     double ibF[3];                /* Ion boundary force */
05829     double npF[3];                /* Non-polar boundary force */
05830
05831     VASSERT(thee != VNULL);
05832
05833     rc = rc && Vpmg_dbForce(thee, qfF, atomID, srfm);
05834     rc = rc && Vpmg_ibForce(thee, dbF, atomID, srfm);
05835     rc = rc && Vpmg_qfForce(thee, ibF, atomID, chgm);
05836
05837     force[0] = qfF[0] + dbF[0] + ibF[0];
05838     force[1] = qfF[1] + dbF[1] + ibF[1];
05839     force[2] = qfF[2] + dbF[2] + ibF[2];
05840
05841     return rc;
05842 }
05843
05844
05845 VPUBLIC int Vpmg_ibForce(Vpmg *thee, double *force, int atomID,
05846     Vsurf_Meth srfm) {
05847
05848     Valist *alist;
05849     Vacc *acc;
05850     Vpbe *pbe;
05851     Vatom *atom;
05852
05853     double *apos, position[3], arad, irad, zkappa2, hx, hy, hzed;
05854     double xlen, ylen, zlen, xmin, ymin, zmin, xmax, ymax, zmax, rtot2;
05855     double rtot, dx, dx2, dy, dy2, dz, dz2, gpos[3], tgrad[3], fmag;
05856     double izmagic;
05857     int i, j, k, nx, ny, nz, imin, imax, jmin, jmax, kmin, kmax;
05858
05859     /* For nonlinear forces */
05860     int ichop, nchop, nion, m;
05861     double ionConc[MAXION], ionRadii[MAXION], ionQ[MAXION], ionstr;
05862
05863     VASSERT(thee != VNULL);
05864
05865     acc = thee->pbe->acc;
05866     atom = Valist_getAtom(thee->pbe->alist, atomID);
05867     apos = Vatom_getPosition(atom);
05868     arad = Vatom_getRadius(atom);
05869
05870     /* Reset force */
05871     force[0] = 0.0;
05872     force[1] = 0.0;
05873     force[2] = 0.0;
05874
05875     /* Check surface definition */
05876     if ((srfm != VSM_SPLINE) && (srfm != VSM_SPLINE3) && (srfm != VSM_SPLINE4)) {
05877         Vnm_print(2, "Vpmg_ibForce: Forces *must* be calculated with \
05878 spline-based surfaces!\n");
05879         Vnm_print(2, "Vpmg_ibForce: Skipping ionic boundary force \
05880 calculation!\n");
05881         return 0;
05882     }
05883
05884     /* If we aren't in the current position, then we're done */
05885     if (atom->partID == 0) return 1;
05886
05887     /* Get PBE info */
05888     pbe = thee->pbe;
05889     acc = pbe->acc;
05890     alist = pbe->alist;
05891     irad = Vpbe_getMaxIonRadius(pbe);
05892     zkappa2 = Vpbe_getZkappa2(pbe);
05893     izmagic = 1.0/Vpbe_getZmagic(pbe);
05894
05895     ionstr = Vpbe_getBulkIonicStrength(pbe);
05896     Vpbe_getIons(pbe, &nion, ionConc, ionRadii, ionQ);
05897
05898     /* Mesh info */
05899     nx = thee->pmgp->nx;
05900     ny = thee->pmgp->ny;
05901     nz = thee->pmgp->nz;
05902     hx = thee->pmgp->hx;
05903     hy = thee->pmgp->hy;
05904     hzed = thee->pmgp->hzed;
05905     xlen = thee->pmgp->xlen;
05906     ylen = thee->pmgp->ylen;
05907     zlen = thee->pmgp->zlen;

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```

05908     xmin = thee->pmpg->xmin;
05909     ymin = thee->pmpg->ymin;
05910     zmin = thee->pmpg->zmin;
05911     xmax = thee->pmpg->xmax;
05912     ymax = thee->pmpg->ymax;
05913     zmax = thee->pmpg->zmax;
05914
05915     /* Sanity check: there is no force if there is zero ionic strength */
05916     if (zkappa2 < VPMGSMALL) {
05917 #ifndef VAPBSQUIET
05918         Vnm_print(2, "Vpmg_ibForce: No force for zero ionic strength!\n");
05919 #endif
05920         return 1;
05921     }
05922
05923     /* Make sure we're on the grid */
05924     if ((apos[0]<=xmin) || (apos[0]>=xmax) || \
05925         (apos[1]<=ymin) || (apos[1]>=ymax) || \
05926         (apos[2]<=zmin) || (apos[2]>=zmax)) {
05927         if ((thee->pmpg->bcfl != BCFL_FOCUS) &&
05928             (thee->pmpg->bcfl != BCFL_MAP)) {
05929             Vnm_print(2, "Vpmg_ibForce: Atom #%d at (%4.3f, %4.3f, %4.3f) is off the mesh (ignoring):\n",
05930                 atom, apos[0], apos[1], apos[2]);
05931             Vnm_print(2, "Vpmg_ibForce:   xmin = %g, xmax = %g\n",
05932                 xmin, xmax);
05933             Vnm_print(2, "Vpmg_ibForce:   ymin = %g, ymax = %g\n",
05934                 ymin, ymax);
05935             Vnm_print(2, "Vpmg_ibForce:   zmin = %g, zmax = %g\n",
05936                 zmin, zmax);
05937         }
05938         fflush(stderr);
05939     } else {
05940
05941         /* Convert the atom position to grid reference frame */
05942         position[0] = apos[0] - xmin;
05943         position[1] = apos[1] - ymin;
05944         position[2] = apos[2] - zmin;
05945
05946         /* Integrate over points within this atom's (inflated) radius */
05947         rtot = (irad + arad + thee->splineWin);
05948         rtot2 = VSQR(rtot);
05949         dx = rtot + 0.5*hx;
05950         imin = VMAX2(0, (int)ceil((position[0] - dx)/hx));
05951         imax = VMIN2(nx-1, (int)floor((position[0] + dx)/hx));
05952         for (i=imin; i<=imax; i++) {
05953             dx2 = VSQR(position[0] - hx*i);
05954             if (rtot2 > dx2) dy = VSQRT(rtot2 - dx2) + 0.5*hy;
05955             else dy = 0.5*hy;
05956             jmin = VMAX2(0, (int)ceil((position[1] - dy)/hy));
05957             jmax = VMIN2(ny-1, (int)floor((position[1] + dy)/hy));
05958             for (j=jmin; j<=jmax; j++) {
05959                 dy2 = VSQR(position[1] - hy*j);
05960                 if (rtot2 > (dx2+dy2)) dz = VSQRT(rtot2-dx2-dy2)+0.5*hzed;
05961                 else dz = 0.5*hzed;
05962                 kmin = VMAX2(0, (int)ceil((position[2] - dz)/hzed));
05963                 kmax = VMIN2(nz-1, (int)floor((position[2] + dz)/hzed));
05964                 for (k=kmin; k<=kmax; k++) {
05965                     dz2 = VSQR(k*hzed - position[2]);
05966                     /* See if grid point is inside ivdw radius and set kappa
05967                      * accordingly (do spline assignment here) */
05968                     if ((dz2 + dy2 + dx2) <= rtot2) {
05969                         gpos[0] = i*hx + xmin;
05970                         gpos[1] = j*hy + ymin;
05971                         gpos[2] = k*hzed + zmin;
05972
05973                         /* Select the correct function based on the surface definition
05974                          * (now including the 7th order polynomial) */
05975                         Vpmg_splineSelect(srff,acc, gpos,thee->splineWin, irad, atom, tgrad);
05976
05977                         if (thee->pmpg->nonlin) {
05978                             /* Nonlinear forces */
05979                             fmag = 0.0;
05980                             nchop = 0;
05981                             for (m=0; m<nion; m++) {
05982                                 fmag +=
05983                                     (thee->kappa[IJK(i,j,k)])*ionConc[m]*(Vcap_exp(-ionQ[m]*thee->u[IJK(i,j,k)], &ichop)-1.0)/ionstr;
05984                                 nchop += ichop;
05985                             }
05986                             /* if (nchop > 0) Vnm_print(2, "Vpmg_ibForece: Chopped EXP %d
05987                                 times!\n", nchop);*/
05988                             force[0] += (zkappa2*fmag*tgrad[0]);

```

```

05987             force[1] += (zkappa2*fmag*tgrad[1]);
05988             force[2] += (zkappa2*fmag*tgrad[2]);
05989         } else {
05990             /* Use of bulk factor (zkappa2) OK here becuae
05991              * LPBE force approximation */
05992             /* NAB -- did we forget a kappa factor here??? */
05993             fmag = VSQR(thee->u[IJK(i,j,k)]*(thee->kappa[IJK(i,j,k)]));
05994             force[0] += (zkappa2*fmag*tgrad[0]);
05995             force[1] += (zkappa2*fmag*tgrad[1]);
05996             force[2] += (zkappa2*fmag*tgrad[2]);
05997         }
05998     }
05999 } /* k loop */
06000 } /* j loop */
06001 } /* i loop */
06002 }
06003 force[0] = force[0] * 0.5 * hx * hy * hzed * izmagic;
06004 force[1] = force[1] * 0.5 * hx * hy * hzed * izmagic;
06005 force[2] = force[2] * 0.5 * hx * hy * hzed * izmagic;
06006
06007 return 1;
06008 }
06009
06010 VPUBLIC int Vpmg_dbForce(Vpmg *thee, double *dbForce, int atomID,
06011                        Vsurf_Meth srfm) {
06012
06013     Vacc *acc;
06014     Vpbe *pbe;
06015     Vatom *atom;
06016
06017     double *apos, position[3], arad, srad, hx, hy, hzed, izmagic, deps, depsi;
06018     double xlen, ylen, zlen, xmin, ymin, zmin, xmax, ymax, zmax, rtot2, epsp;
06019     double rtot, dx, gpos[3], tgrad[3], dbFmag, epsw, kT;
06020     double *u, Hxijk, Hyijk, Hzij, Hximljk, Hyijmlk, Hzijkm1;
06021     double dHxijk[3], dHyijk[3], dHzij[3], dHximljk[3], dHyijmlk[3];
06022     double dHzijkm1[3];
06023     int i, j, k, l, nx, ny, nz, imin, imax, jmin, jmax, kmin, kmax;
06024
06025     VASSERT(thee != VNULL);
06026     if (!thee->filled) {
06027         Vnm_print(2, "Vpmg_dbForce: Need to callVpmg_fillco!\n");
06028         return 0;
06029     }
06030
06031     acc = thee->pbe->acc;
06032     atom = Valist_getAtom(thee->pbe->alist, atomID);
06033     apos = Vatom_getPosition(atom);
06034     arad = Vatom_getRadius(atom);
06035     srad = Vpbe_getSolventRadius(thee->pbe);
06036
06037     /* Reset force */
06038     dbForce[0] = 0.0;
06039     dbForce[1] = 0.0;
06040     dbForce[2] = 0.0;
06041
06042     /* Check surface definition */
06043     if ((srfm != VSM_SPLINE) && (srfm != VSM_SPLINE3) && (srfm != VSM_SPLINE4)) {
06044         Vnm_print(2, "Vpmg_dbForce: Forces *must* be calculated with \
06045 spline-based surfaces!\n");
06046         Vnm_print(2, "Vpmg_dbForce: Skipping dielectric/apolar boundary \
06047 force calculation!\n");
06048         return 0;
06049     }
06050
06051     /* If we aren't in the current position, then we're done */
06052     if (atom->partID == 0) return 1;
06053
06054     /* Get PBE info */
06055     pbe = thee->pbe;
06056     acc = pbe->acc;
06057     epsp = Vpbe_getSoluteDiel(pbe);
06058     epsw = Vpbe_getSolventDiel(pbe);
06059     kT = Vpbe_getTemperature(pbe) * (1e-3) * Vunit_Na * Vunit_kb;
06060     izmagic = 1.0 / Vpbe_getZmagic(pbe);
06061
06062     /* Mesh info */
06063     nx = thee->pmgp->nx;
06064     ny = thee->pmgp->ny;
06065     nz = thee->pmgp->nz;
06066     hx = thee->pmgp->hx;

```



```

06068     hy = thee->pmgp->hy;
06069     hzed = thee->pmgp->hzcd;
06070     xlen = thee->pmgp->xlen;
06071     ylen = thee->pmgp->ylen;
06072     zlen = thee->pmgp->zlen;
06073     xmin = thee->pmgp->xmin;
06074     ymin = thee->pmgp->ymin;
06075     zmin = thee->pmgp->zmin;
06076     xmax = thee->pmgp->xmax;
06077     ymax = thee->pmgp->ymax;
06078     zmax = thee->pmgp->zmax;
06079     u = thee->u;
06080
06081     /* Sanity check: there is no force if there is zero ionic strength */
06082     if (VABS(epsw-eps) < VPMGSMALL) {
06083         Vnm_print(0, "Vpmg_dbForce: No force for uniform dielectric!\n");
06084         return 1;
06085     }
06086     deps = (epsw - eps);
06087     depsi = 1.0/deps;
06088     rtot = (arad + thee->splineWin + srads);
06089
06090     /* Make sure we're on the grid */
06091     /* Grid checking modified by Matteo Rotter */
06092     if ((apos[0]<=xmin + rtot) || (apos[0]>=xmax - rtot) || \
06093         (apos[1]<=ymin + rtot) || (apos[1]>=ymax - rtot) || \
06094         (apos[2]<=zmin + rtot) || (apos[2]>=zmax - rtot)) {
06095         if ((thee->pmgp->bcfl != BCFL_FOCUS) &&
06096             (thee->pmgp->bcfl != BCFL_MAP)) {
06097             Vnm_print(2, "Vpmg_dbForce: Atom #%d at (%4.3f, %4.3f, %4.3f) is off the mesh (ignoring):\n",
06098                 atomID, apos[0], apos[1], apos[2]);
06099             Vnm_print(2, "Vpmg_dbForce:      xmin = %g, xmax = %g\n",
06100                 xmin, xmax);
06101             Vnm_print(2, "Vpmg_dbForce:      ymin = %g, ymax = %g\n",
06102                 ymin, ymax);
06103             Vnm_print(2, "Vpmg_dbForce:      zmin = %g, zmax = %g\n",
06104                 zmin, zmax);
06105         }
06106         fflush(stderr);
06107     } else {
06108
06109         /* Convert the atom position to grid reference frame */
06110         position[0] = apos[0] - xmin;
06111         position[1] = apos[1] - ymin;
06112         position[2] = apos[2] - zmin;
06113
06114         /* Integrate over points within this atom's (inflated) radius */
06115         rtot2 = VSQR(rtot);
06116         dx = rtot/hx;
06117         imin = (int)floor((position[0]-rtot)/hx);
06118         if (imin < 1) {
06119             Vnm_print(2, "Vpmg_dbForce: Atom %d off grid!\n", atomID);
06120             return 0;
06121         }
06122         imax = (int)ceil((position[0]+rtot)/hx);
06123         if (imax > (nx-2)) {
06124             Vnm_print(2, "Vpmg_dbForce: Atom %d off grid!\n", atomID);
06125             return 0;
06126         }
06127         jmin = (int)floor((position[1]-rtot)/hy);
06128         if (jmin < 1) {
06129             Vnm_print(2, "Vpmg_dbForce: Atom %d off grid!\n", atomID);
06130             return 0;
06131         }
06132         jmax = (int)ceil((position[1]+rtot)/hy);
06133         if (jmax > (ny-2)) {
06134             Vnm_print(2, "Vpmg_dbForce: Atom %d off grid!\n", atomID);
06135             return 0;
06136         }
06137         kmin = (int)floor((position[2]-rtot)/hzcd);
06138         if (kmin < 1) {
06139             Vnm_print(2, "Vpmg_dbForce: Atom %d off grid!\n", atomID);
06140             return 0;
06141         }
06142         kmax = (int)ceil((position[2]+rtot)/hzcd);
06143         if (kmax > (nz-2)) {
06144             Vnm_print(2, "Vpmg_dbForce: Atom %d off grid!\n", atomID);
06145             return 0;
06146         }
06147         for (i=imin; i<=imax; i++) {
06148             for (j=jmin; j<=jmax; j++) {

```

```

06149         for (k=kmin; k<=kmax; k++) {
06150             /* i,j,k */
06151             gpos[0] = (i+0.5)*hx + xmin;
06152             gpos[1] = j*hy + ymin;
06153             gpos[2] = k*hzed + zmin;
06154             Hxijk = (thee->epsx[IJK(i,j,k)] - epsp)*depsi;
06155
06156             /* Select the correct function based on the surface definition
06157              * (now including the 7th order polynomial) */
06158             Vpmg_splineSelect(srfm,acc, gpos, thee->splineWin, 0.,atom, dHxijk);
06159             /*
06160              switch (srfm) {
06161                  case VSM_SPLINE :
06162                      Vacc_splineAccGradAtomNorm(acc, gpos, thee->splineWin, 0.,
06163                                                  atom, dHxijk);
06164                      break;
06165                  case VSM_SPLINE4 :
06166                      Vacc_splineAccGradAtomNorm4(acc, gpos, thee->splineWin, 0.,
06167                                                  atom, dHxijk);
06168                      break;
06169                  default:
06170                      Vnm_print(2, "Vpmg_dbnbForce: Unknown surface method.\n");
06171                      return;
06172              }
06173             */
06174             for (l=0; l<3; l++) dHxijk[l] *= Hxijk;
06175             gpos[0] = i*hx + xmin;
06176             gpos[1] = (j+0.5)*hy + ymin;
06177             gpos[2] = k*hzed + zmin;
06178             Hyijk = (thee->epsy[IJK(i,j,k)] - epsp)*depsi;
06179
06180             /* Select the correct function based on the surface definition
06181              * (now including the 7th order polynomial) */
06182             Vpmg_splineSelect(srfm,acc, gpos, thee->splineWin, 0.,atom, dHyijk);
06183
06184             for (l=0; l<3; l++) dHyijk[l] *= Hyijk;
06185             gpos[0] = i*hx + xmin;
06186             gpos[1] = j*hy + ymin;
06187             gpos[2] = (k+0.5)*hzed + zmin;
06188             Hzijk = (thee->epsz[IJK(i,j,k)] - epsp)*depsi;
06189
06190             /* Select the correct function based on the surface definition
06191              * (now including the 7th order polynomial) */
06192             Vpmg_splineSelect(srfm,acc, gpos, thee->splineWin, 0.,atom, dHzijk);
06193
06194             for (l=0; l<3; l++) dHzijk[l] *= Hzijk;
06195             /* i-1,j,k */
06196             gpos[0] = (i-0.5)*hx + xmin;
06197             gpos[1] = j*hy + ymin;
06198             gpos[2] = k*hzed + zmin;
06199             Hximljk = (thee->epsx[IJK(i-1,j,k)] - epsp)*depsi;
06200
06201             /* Select the correct function based on the surface definition
06202              * (now including the 7th order polynomial) */
06203             Vpmg_splineSelect(srfm,acc, gpos, thee->splineWin, 0.,atom, dHximljk);
06204
06205             for (l=0; l<3; l++) dHximljk[l] *= Hximljk;
06206             /* i,j-1,k */
06207             gpos[0] = i*hx + xmin;
06208             gpos[1] = (j-0.5)*hy + ymin;
06209             gpos[2] = k*hzed + zmin;
06210             Hyijmlk = (thee->epsy[IJK(i,j-1,k)] - epsp)*depsi;
06211
06212             /* Select the correct function based on the surface definition
06213              * (now including the 7th order polynomial) */
06214             Vpmg_splineSelect(srfm,acc, gpos, thee->splineWin, 0.,atom, dHyijmlk);
06215
06216             for (l=0; l<3; l++) dHyijmlk[l] *= Hyijmlk;
06217             /* i,j,k-1 */
06218             gpos[0] = i*hx + xmin;
06219             gpos[1] = j*hy + ymin;
06220             gpos[2] = (k-0.5)*hzed + zmin;
06221             Hzijkml = (thee->epsz[IJK(i,j,k-1)] - epsp)*depsi;
06222
06223             /* Select the correct function based on the surface definition
06224              * (now including the 7th order polynomial) */
06225             Vpmg_splineSelect(srfm,acc, gpos, thee->splineWin, 0.,atom, dHzijkml);
06226
06227             for (l=0; l<3; l++) dHzijkml[l] *= Hzijkml;
06228             /* *** CALCULATE DIELECTRIC BOUNDARY FORCES *** */
06229             dbFmag = u[IJK(i,j,k)];

```

```

06230         tgrad[0] =
06231             (dHxijk[0] * (u[IJK(i+1,j,k)]-u[IJK(i,j,k)]))
06232             + dHximljk[0] * (u[IJK(i-1,j,k)]-u[IJK(i,j,k)])) /VSQR(hx)
06233             + (dHyijk[0] * (u[IJK(i,j+1,k)]-u[IJK(i,j,k)]))
06234             + dHyijmlk[0] * (u[IJK(i,j-1,k)]-u[IJK(i,j,k)])) /VSQR(hy)
06235             + (dHzijk[0] * (u[IJK(i,j,k+1)]-u[IJK(i,j,k)]))
06236             + dHzijkml[0] * (u[IJK(i,j,k-1)]-u[IJK(i,j,k)])) /VSQR(hzed);
06237         tgrad[1] =
06238             (dHxijk[1] * (u[IJK(i+1,j,k)]-u[IJK(i,j,k)]))
06239             + dHximljk[1] * (u[IJK(i-1,j,k)]-u[IJK(i,j,k)])) /VSQR(hx)
06240             + (dHyijk[1] * (u[IJK(i,j+1,k)]-u[IJK(i,j,k)]))
06241             + dHyijmlk[1] * (u[IJK(i,j-1,k)]-u[IJK(i,j,k)])) /VSQR(hy)
06242             + (dHzijk[1] * (u[IJK(i,j,k+1)]-u[IJK(i,j,k)]))
06243             + dHzijkml[1] * (u[IJK(i,j,k-1)]-u[IJK(i,j,k)])) /VSQR(hzed);
06244         tgrad[2] =
06245             (dHxijk[2] * (u[IJK(i+1,j,k)]-u[IJK(i,j,k)]))
06246             + dHximljk[2] * (u[IJK(i-1,j,k)]-u[IJK(i,j,k)])) /VSQR(hx)
06247             + (dHyijk[2] * (u[IJK(i,j+1,k)]-u[IJK(i,j,k)]))
06248             + dHyijmlk[2] * (u[IJK(i,j-1,k)]-u[IJK(i,j,k)])) /VSQR(hy)
06249             + (dHzijk[2] * (u[IJK(i,j,k+1)]-u[IJK(i,j,k)]))
06250             + dHzijkml[2] * (u[IJK(i,j,k-1)]-u[IJK(i,j,k)])) /VSQR(hzed);
06251         dbForce[0] += (dbFmag*tgrad[0]);
06252         dbForce[1] += (dbFmag*tgrad[1]);
06253         dbForce[2] += (dbFmag*tgrad[2]);
06254     } /* k loop */
06255 } /* j loop */
06256 } /* i loop */
06257
06258     dbForce[0] = -dbForce[0]*hx*hy*hzed*deps*0.5*izmagic;
06259     dbForce[1] = -dbForce[1]*hx*hy*hzed*deps*0.5*izmagic;
06260     dbForce[2] = -dbForce[2]*hx*hy*hzed*deps*0.5*izmagic;
06261 }
06262
06263     return 1;
06264 }
06265
06266
06267 VPUBLIC int Vpmg_qfForce(Vpmg *thee, double *force, int atomID,
06268     Vchrg_Meth chgm) {
06269     double tforce[3];
06270
06271     /* Reset force */
06272     force[0] = 0.0;
06273     force[1] = 0.0;
06274     force[2] = 0.0;
06275
06276     /* Check surface definition */
06277     if (chgm != VCM_BSPL2) {
06278         Vnm_print(2, "Vpmg_qfForce: It is recommended that forces be \
06279 calculated with the\n");
06280         Vnm_print(2, "Vpmg_qfForce: cubic spline charge discretization \
06281 scheme\n");
06282     }
06283
06284     switch (chgm) {
06285     case VCM_TRIL:
06286         qfForceSpline1(thee, tforce, atomID);
06287         break;
06288     case VCM_BSPL2:
06289         qfForceSpline2(thee, tforce, atomID);
06290         break;
06291     case VCM_BSPL4:
06292         qfForceSpline4(thee, tforce, atomID);
06293         break;
06294     default:
06295         Vnm_print(2, "Vpmg_qfForce: Undefined charge discretization \
06296 method (%d)!\n", chgm);
06297         Vnm_print(2, "Vpmg_qfForce: Forces not calculated!\n");
06298         return 0;
06299     }
06300
06301     /* Assign forces */
06302     force[0] = tforce[0];
06303     force[1] = tforce[1];
06304     force[2] = tforce[2];
06305
06306     return 1;
06307 }
06308
06309
06310

```

```

06311 VPRIVATE void qfForceSpline1(Vpmg *thee, double *force, int atomID) {
06312
06313     Vatom *atom;
06314
06315     double *apos, position[3], hx, hy, hzed;
06316     double xmin, ymin, zmin, xmax, ymax, zmax;
06317     double dx, dy, dz;
06318     double *u, charge, ifloat, jfloat, kfloat;
06319     int nx, ny, nz, ihi, ilo, jhi, jlo, khi, klo;
06320
06321     VASSERT(thee != VNULL);
06322
06323     atom = Valist_getAtom(thee->pbe->alist, atomID);
06324     apos = Vatom_getPosition(atom);
06325     charge = Vatom_getCharge(atom);
06326
06327     /* Reset force */
06328     force[0] = 0.0;
06329     force[1] = 0.0;
06330     force[2] = 0.0;
06331
06332     /* If we aren't in the current position, then we're done */
06333     if (atom->partID == 0) return;
06334
06335     /* Mesh info */
06336     nx = thee->pmgp->nx;
06337     ny = thee->pmgp->ny;
06338     nz = thee->pmgp->nz;
06339     hx = thee->pmgp->hx;
06340     hy = thee->pmgp->hy;
06341     hzed = thee->pmgp->hzed;
06342     xmin = thee->pmgp->xmin;
06343     ymin = thee->pmgp->ymin;
06344     zmin = thee->pmgp->zmin;
06345     xmax = thee->pmgp->xmax;
06346     ymax = thee->pmgp->ymax;
06347     zmax = thee->pmgp->zmax;
06348     u = thee->u;
06349
06350     /* Make sure we're on the grid */
06351     if ((apos[0]<=xmin) || (apos[0]>=xmax) || (apos[1]<=ymin) || \
06352         (apos[1]>=ymax) || (apos[2]<=zmin) || (apos[2]>=zmax)) {
06353         if ((thee->pmgp->bcfl != BCFL_FOCUS) &&
06354             (thee->pmgp->bcfl != BCFL_MAP)) {
06355             Vnm_print(2, "Vpmg_qfForce: Atom #d at (%4.3f, %4.3f, %4.3f) is off the mesh (ignoring):\n",
atomID, apos[0], apos[1], apos[2]);
06356             Vnm_print(2, "Vpmg_qfForce:      xmin = %g, xmax = %g\n", xmin, xmax);
06357             Vnm_print(2, "Vpmg_qfForce:      ymin = %g, ymax = %g\n", ymin, ymax);
06358             Vnm_print(2, "Vpmg_qfForce:      zmin = %g, zmax = %g\n", zmin, zmax);
06359         }
06360         fflush(stderr);
06361     } else {
06362
06363         /* Convert the atom position to grid coordinates */
06364         position[0] = apos[0] - xmin;
06365         position[1] = apos[1] - ymin;
06366         position[2] = apos[2] - zmin;
06367         ifloat = position[0]/hx;
06368         jfloat = position[1]/hy;
06369         kfloat = position[2]/hzed;
06370         ihi = (int)ceil(ifloat);
06371         ilo = (int)floor(ifloat);
06372         jhi = (int)ceil(jfloat);
06373         jlo = (int)floor(jfloat);
06374         khi = (int)ceil(kfloat);
06375         klo = (int)floor(kfloat);
06376         VASSERT((ihi < nx) && (ihi >=0));
06377         VASSERT((ilo < nx) && (ilo >=0));
06378         VASSERT((jhi < ny) && (jhi >=0));
06379         VASSERT((jlo < ny) && (jlo >=0));
06380         VASSERT((khi < nz) && (khi >=0));
06381         VASSERT((klo < nz) && (klo >=0));
06382         dx = ifloat - (double)(ilo);
06383         dy = jfloat - (double)(jlo);
06384         dz = kfloat - (double)(klo);
06385
06386
06387     #if 0
06388         Vnm_print(1, "Vpmg_qfForce: (DEBUG) u ~ %g\n",
06389             dx      *dy      *dz      *u[IJK(ihi,jhi,khi)]
06390             +dx      *dy      *(1-dz) *u[IJK(ihi,jhi,klo)]

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```

06391     +dx     *(1-dy)*dz     *u[IJK(ihi,jlo,khi)]
06392     +dx     *(1-dy)*(1-dz)*u[IJK(ihi,jlo,klo)]
06393     + (1-dx)*dy     *dz     *u[IJK(ilo,jhi,khi)]
06394     + (1-dx)*dy     *(1-dz)*u[IJK(ilo,jhi,klo)]
06395     + (1-dx)*(1-dy)*dz     *u[IJK(ilo,jlo,khi)]
06396     + (1-dx)*(1-dy)*(1-dz)*u[IJK(ilo,jlo,klo)];
06397 #endif
06398
06399
06400     if ((dx > VPMGSMALL) && (VABS(1.0-dx) > VPMGSMALL)) {
06401         force[0] =
06402             -charge*(dy     *dz     *u[IJK(ihi,jhi,khi)]
06403                 + dy     *(1-dz)*u[IJK(ihi,jhi,klo)]
06404                 + (1-dy)*dz     *u[IJK(ihi,jlo,khi)]
06405                 + (1-dy)*(1-dz)*u[IJK(ihi,jlo,klo)]
06406                 - dy     *dz     *u[IJK(ilo,jhi,khi)]
06407                 - dy     *(1-dz)*u[IJK(ilo,jhi,klo)]
06408                 - (1-dy)*dz     *u[IJK(ilo,jlo,khi)]
06409                 - (1-dy)*(1-dz)*u[IJK(ilo,jlo,klo)])/hx;
06410     } else {
06411         force[0] = 0;
06412         Vnm_print(0,
06413             "Vpmg_qfForce: Atom %d on x gridline; zero x-force\n", atomID);
06414     }
06415     if ((dy > VPMGSMALL) && (VABS(1.0-dy) > VPMGSMALL)) {
06416         force[1] =
06417             -charge*(dx     *dz     *u[IJK(ihi,jhi,khi)]
06418                 + dx     *(1-dz)*u[IJK(ihi,jhi,klo)]
06419                 - dx     *dz     *u[IJK(ihi,jlo,khi)]
06420                 - dx     *(1-dz)*u[IJK(ihi,jlo,klo)]
06421                 + (1-dx)*dz     *u[IJK(ilo,jhi,khi)]
06422                 + (1-dx)*(1-dz)*u[IJK(ilo,jhi,klo)]
06423                 - (1-dx)*dz     *u[IJK(ilo,jlo,khi)]
06424                 - (1-dx)*(1-dz)*u[IJK(ilo,jlo,klo)])/hy;
06425     } else {
06426         force[1] = 0;
06427         Vnm_print(0,
06428             "Vpmg_qfForce: Atom %d on y gridline; zero y-force\n", atomID);
06429     }
06430     if ((dz > VPMGSMALL) && (VABS(1.0-dz) > VPMGSMALL)) {
06431         force[2] =
06432             -charge*(dy     *dx     *u[IJK(ihi,jhi,khi)]
06433                 - dy     *dx     *u[IJK(ihi,jhi,klo)]
06434                 + (1-dy)*dx     *u[IJK(ihi,jlo,khi)]
06435                 - (1-dy)*dx     *u[IJK(ihi,jlo,klo)]
06436                 + dy     *(1-dx)*u[IJK(ilo,jhi,khi)]
06437                 - dy     *(1-dx)*u[IJK(ilo,jhi,klo)]
06438                 + (1-dy)*(1-dx)*u[IJK(ilo,jlo,khi)]
06439                 - (1-dy)*(1-dx)*u[IJK(ilo,jlo,klo)])/hz;
06440     } else {
06441         force[2] = 0;
06442         Vnm_print(0,
06443             "Vpmg_qfForce: Atom %d on z gridline; zero z-force\n", atomID);
06444     }
06445 }
06446 }
06447
06448 VPRIVATE void qfForceSpline2(Vpmg *thee, double *force, int atomID) {
06449
06450     Vatom *atom;
06451
06452     double *apos, position[3], hx, hy, hzed;
06453     double xlen, ylen, zlen, xmin, ymin, zmin, xmax, ymax, zmax;
06454     double mx, my, mz, dmx, dmy, dmz;
06455     double *u, charge, ifloat, jfloat, kfloat;
06456     int nx, ny, nz, im2, im1, ip1, ip2, jm2, jml, jp1, jp2, km2, kml;
06457     int kp1, kp2, ii, jj, kk;
06458
06459     VASSERT(thee != VNULL);
06460
06461     atom = Valist_getAtom(thee->pbe->alist, atomID);
06462     apos = Vatom_getPosition(atom);
06463     charge = Vatom_getCharge(atom);
06464
06465     /* Reset force */
06466     force[0] = 0.0;
06467     force[1] = 0.0;
06468     force[2] = 0.0;
06469
06470     /* If we aren't in the current position, then we're done */
06471     if (atom->partID == 0) return;

```

```

06472
06473 /* Mesh info */
06474 nx = thee->pmgp->nx;
06475 ny = thee->pmgp->ny;
06476 nz = thee->pmgp->nz;
06477 hx = thee->pmgp->hx;
06478 hy = thee->pmgp->hy;
06479 hzed = thee->pmgp->hzed;
06480 xlen = thee->pmgp->xlen;
06481 ylen = thee->pmgp->ylen;
06482 zlen = thee->pmgp->zlen;
06483 xmin = thee->pmgp->xmin;
06484 ymin = thee->pmgp->ymin;
06485 zmin = thee->pmgp->zmin;
06486 xmax = thee->pmgp->xmax;
06487 ymax = thee->pmgp->ymax;
06488 zmax = thee->pmgp->zmax;
06489 u = thee->u;
06490
06491 /* Make sure we're on the grid */
06492 if ((apos[0] <= (xmin+hx)) || (apos[0] >= (xmax-hx)) \
06493 || (apos[1] <= (ymin+hy)) || (apos[1] >= (ymax-hy)) \
06494 || (apos[2] <= (zmin+hzed)) || (apos[2] >= (zmax-hzed))) {
06495     if ((thee->pmgp->bcfl != BCFL_FOCUS) &&
06496         (thee->pmgp->bcfl != BCFL_MAP)) {
06497         Vnm_print(2, "qfForceSpline2: Atom #%d off the mesh \
06498             (ignoring)\n", atomID);
06499     }
06500     fflush(stderr);
06501 } else {
06502
06503     /* Convert the atom position to grid coordinates */
06504     position[0] = apos[0] - xmin;
06505     position[1] = apos[1] - ymin;
06506     position[2] = apos[2] - zmin;
06507     ifloat = position[0]/hx;
06508     jfloat = position[1]/hy;
06509     kfloat = position[2]/hzed;
06510     ip1 = (int)ceil(ifloat);
06511     ip2 = ip1 + 1;
06512     im1 = (int)floor(ifloat);
06513     im2 = im1 - 1;
06514     jp1 = (int)ceil(jfloat);
06515     jp2 = jp1 + 1;
06516     jm1 = (int)floor(jfloat);
06517     jm2 = jm1 - 1;
06518     kp1 = (int)ceil(kfloat);
06519     kp2 = kp1 + 1;
06520     km1 = (int)floor(kfloat);
06521     km2 = km1 - 1;
06522
06523     /* This step shouldn't be necessary, but it saves nasty debugging
06524      * later on if something goes wrong */
06525     ip2 = VMIN2(ip2,nx-1);
06526     ip1 = VMIN2(ip1,nx-1);
06527     im1 = VMAX2(im1,0);
06528     im2 = VMAX2(im2,0);
06529     jp2 = VMIN2(jp2,ny-1);
06530     jp1 = VMIN2(jp1,ny-1);
06531     jm1 = VMAX2(jm1,0);
06532     jm2 = VMAX2(jm2,0);
06533     kp2 = VMIN2(kp2,nz-1);
06534     kp1 = VMIN2(kp1,nz-1);
06535     km1 = VMAX2(km1,0);
06536     km2 = VMAX2(km2,0);
06537
06538     for (ii=im2; ii<=ip2; ii++) {
06539         mx = bspline2(VFCHI(ii,ifloat));
06540         dmx = dbspline2(VFCHI(ii,ifloat));
06541         for (jj=jm2; jj<=jp2; jj++) {
06542             my = bspline2(VFCHI(jj,jfloat));
06543             dmy = dbspline2(VFCHI(jj,jfloat));
06544             for (kk=km2; kk<=kp2; kk++) {
06545                 mz = bspline2(VFCHI(kk,kfloat));
06546                 dmz = dbspline2(VFCHI(kk,kfloat));
06547
06548                 force[0] += (charge*dmx*my*mz*u[IJK(ii,jj,kk)])/hx;
06549                 force[1] += (charge*mx*dmy*mz*u[IJK(ii,jj,kk)])/hy;
06550                 force[2] += (charge*mx*my*dmz*u[IJK(ii,jj,kk)])/hzed;
06551             }
06552         }
06553     }

```

```

06553     }
06554     }
06555     }
06556     }
06557     }
06558     }
06559 }
06560
06561 VPRIVATE void qfForceSpline4(Vpmg *thee, double *force, int atomID) {
06562     Vatom *atom;
06563     double f, c, *u, *apos, position[3];
06564
06565     /* Grid variables */
06566     int nx,ny,nz;
06567     double xlen, ylen, zlen, xmin, ymin, zmin, xmax, ymax, zmax;
06568     double hx, hy, hzed, ifloat, jfloat, kfloat;
06569
06570     /* B-spline weights */
06571     double mx, my, mz, dmX, dmy, dmz;
06572     double mi, mj, mk;
06573
06574     /* Loop indeces */
06575     int i, j, k, ii, jj, kk;
06576     int im2, im1, ip1, ip2, jm2, jm1, jp1, jp2, km2, km1, kp1, kp2;
06577
06578     /* field */
06579     double e[3];
06580
06581     VASSERT(thee != VNULL);
06582     VASSERT(thee->filled);
06583
06584     atom = Valist_getAtom(thee->pbe->alist, atomID);
06585     apos = Vatom_getPosition(atom);
06586     c = Vatom_getCharge(atom);
06587
06588     for (i=0;i<3;i++){
06589         e[i] = 0.0;
06590     }
06591
06592     /* Mesh info */
06593     nx = thee->pmgp->nx;
06594     ny = thee->pmgp->ny;
06595     nz = thee->pmgp->nz;
06596     hx = thee->pmgp->hx;
06597     hy = thee->pmgp->hy;
06598     hzed = thee->pmgp->hzed;
06599     xlen = thee->pmgp->xlen;
06600     ylen = thee->pmgp->ylen;
06601     zlen = thee->pmgp->zlen;
06602     xmin = thee->pmgp->xmin;
06603     ymin = thee->pmgp->ymin;
06604     zmin = thee->pmgp->zmin;
06605     xmax = thee->pmgp->xmax;
06606     ymax = thee->pmgp->ymax;
06607     zmax = thee->pmgp->zmax;
06608     u = thee->u;
06609
06610     /* Make sure we're on the grid */
06611     if ((apos[0]<=(xmin+2*hx)) || (apos[0]>=(xmax-2*hx)) \
06612         || (apos[1]<=(ymin+2*hy)) || (apos[1]>=(ymax-2*hy)) \
06613         || (apos[2]<=(zmin+2*hzed)) || (apos[2]>=(zmax-2*hzed))) {
06614         Vnm_print(2, "qfForceSpline4: Atom off the mesh \
06615             (ignoring) %6.3f %6.3f %6.3f\n", apos[0], apos[1], apos[2]);
06616         fflush(stderr);
06617     } else {
06618
06619         /* Convert the atom position to grid coordinates */
06620         position[0] = apos[0] - xmin;
06621         position[1] = apos[1] - ymin;
06622         position[2] = apos[2] - zmin;
06623         ifloat = position[0]/hx;
06624         jfloat = position[1]/hy;
06625         kfloat = position[2]/hzed;
06626         ip1 = (int)ceil(ifloat);
06627         ip2 = ip1 + 2;
06628         im1 = (int)floor(ifloat);
06629         im2 = im1 - 2;
06630         jp1 = (int)ceil(jfloat);
06631         jp2 = jp1 + 2;
06632         jm1 = (int)floor(jfloat);

```

```

06634         jm2 = jm1 - 2;
06635         kp1 = (int)ceil(kfloat);
06636         kp2 = kp1 + 2;
06637         km1 = (int)floor(kfloat);
06638         km2 = km1 - 2;
06639
06640         /* This step shouldn't be necessary, but it saves nasty debugging
06641          * later on if something goes wrong */
06642         ip2 = VMIN2(ip2,nx-1);
06643         ip1 = VMIN2(ip1,nx-1);
06644         im1 = VMAX2(im1,0);
06645         im2 = VMAX2(im2,0);
06646         jp2 = VMIN2(jp2,ny-1);
06647         jp1 = VMIN2(jp1,ny-1);
06648         jm1 = VMAX2(jm1,0);
06649         jm2 = VMAX2(jm2,0);
06650         kp2 = VMIN2(kp2,nz-1);
06651         kp1 = VMIN2(kp1,nz-1);
06652         km1 = VMAX2(km1,0);
06653         km2 = VMAX2(km2,0);
06654
06655         for (ii=im2; ii<=ip2; ii++) {
06656             mi = VFCHI4(ii,ifloat);
06657             mx = bspline4(mi);
06658             dmx = dbspline4(mi);
06659             for (jj=jm2; jj<=jp2; jj++) {
06660                 mj = VFCHI4(jj,jfloat);
06661                 my = bspline4(mj);
06662                 dmy = dbspline4(mj);
06663                 for (kk=km2; kk<=kp2; kk++) {
06664                     mk = VFCHI4(kk,kfloat);
06665                     mz = bspline4(mk);
06666                     dmz = dbspline4(mk);
06667                     f = u[IJK(ii,jj,kk)];
06668                     /* Field */
06669                     e[0] += f*dmx*my*mz/hx;
06670                     e[1] += f*mx*dmy*mz/hy;
06671                     e[2] += f*mx*my*dmz/hzed;
06672                 }
06673             }
06674         }
06675     }
06676
06677     /* Monopole Force */
06678     force[0] = e[0]*c;
06679     force[1] = e[1]*c;
06680     force[2] = e[2]*c;
06681
06682 }
06683
06684 VPRIVATE void markFrac(
06685     double rtot, double *tpos,
06686     int nx, int ny, int nz,
06687     double hx, double hy, double hzed,
06688     double xmin, double ymin, double zmin,
06689     double *xarray, double *yarray, double *zarray) {
06690
06691     int i, j, k, imin, imax, jmin, jmax, kmin, kmax;
06692     double dx, dx2, dy, dy2, dz, dz2, a000, a001, a010, a100, r2;
06693     double x, xp, xm, y, yp, ym, zp, z, zm, xspan, yspan, zspan;
06694     double rtot2, pos[3];
06695
06696     /* Convert to grid reference frame */
06697     pos[0] = tpos[0] - xmin;
06698     pos[1] = tpos[1] - ymin;
06699     pos[2] = tpos[2] - zmin;
06700
06701     rtot2 = VSQR(rtot);
06702
06703     xspan = rtot + 2*hx;
06704     imin = VMAX2(0, (int)ceil((pos[0] - xspan)/hx));
06705     imax = VMIN2(nx-1, (int)floor((pos[0] + xspan)/hx));
06706     for (i=imin; i<=imax; i++) {
06707         x = hx*i;
06708         dx2 = VSQR(pos[0] - x);
06709         if (rtot2 > dx2) {
06710             yspan = VSQRT(rtot2 - dx2) + 2*hy;
06711         } else {
06712             yspan = 2*hy;
06713         }
06714         jmin = VMAX2(0, (int)ceil((pos[1] - yspan)/hy));

```



```

06715     jmax = VMIN2(ny-1, (int)floor((pos[1] + yspan)/hy));
06716     for (j=jmin; j<=jmax; j++) {
06717         y = hy*j;
06718         dy2 = VSQR(pos[1] - y);
06719         if (rtot2 > (dx2+dy2)) {
06720             zspan = VSQRT(rtot2-dx2-dy2) + 2*hzed;
06721         } else {
06722             zspan = 2*hzed;
06723         }
06724         kmin = VMAX2(0, (int)ceil((pos[2] - zspan)/hzed));
06725         kmax = VMIN2(nz-1, (int)floor((pos[2] + zspan)/hzed));
06726         for (k=kmin; k<=kmax; k++) {
06727             z = hzed*k;
06728             dz2 = VSQR(pos[2] - z);
06729
06730             r2 = dx2 + dy2 + dz2;
06731
06732             /* We need to determine the inclusion value a000 at (i,j,k) */
06733             if (r2 < rtot2) a000 = 1.0;
06734             else a000 = 0.0;
06735
06736             /* We need to evaluate the values of x which intersect the
06737              * sphere and determine if these are in the interval
06738              * [(i,j,k), (i+1,j,k)] */
06739             if (r2 < (rtot2 - hx*hx)) a100 = 1.0;
06740             else if (r2 > (rtot2 + hx*hx)) a100 = 0.0;
06741             else if (rtot2 > (dy2 + dz2)) {
06742                 dx = VSQRT(rtot2 - dy2 - dz2);
06743                 xm = pos[0] - dx;
06744                 xp = pos[0] + dx;
06745                 if ((xm < x+hx) && (xm > x)) {
06746                     a100 = (xm - x)/hx;
06747                 } else if ((xp < x+hx) && (xp > x)) {
06748                     a100 = (xp - x)/hx;
06749                 }
06750             } else a100 = 0.0;
06751
06752             /* We need to evaluate the values of y which intersect the
06753              * sphere and determine if these are in the interval
06754              * [(i,j,k), (i,j+1,k)] */
06755             if (r2 < (rtot2 - hy*hy)) a010 = 1.0;
06756             else if (r2 > (rtot2 + hy*hy)) a010 = 0.0;
06757             else if (rtot2 > (dx2 + dz2)) {
06758                 dy = VSQRT(rtot2 - dx2 - dz2);
06759                 ym = pos[1] - dy;
06760                 yp = pos[1] + dy;
06761                 if ((ym < y+hy) && (ym > y)) {
06762                     a010 = (ym - y)/hy;
06763                 } else if ((yp < y+hy) && (yp > y)) {
06764                     a010 = (yp - y)/hy;
06765                 }
06766             } else a010 = 0.0;
06767
06768             /* We need to evaluate the values of y which intersect the
06769              * sphere and determine if these are in the interval
06770              * [(i,j,k), (i,j,k+1)] */
06771             if (r2 < (rtot2 - hzed*hzed)) a001 = 1.0;
06772             else if (r2 > (rtot2 + hzed*hzed)) a001 = 0.0;
06773             else if (rtot2 > (dx2 + dy2)) {
06774                 dz = VSQRT(rtot2 - dx2 - dy2);
06775                 zm = pos[2] - dz;
06776                 zp = pos[2] + dz;
06777                 if ((zm < z+hzed) && (zm > z)) {
06778                     a001 = (zm - z)/hzed;
06779                 } else if ((zp < z+hzed) && (zp > z)) {
06780                     a001 = (zp - z)/hzed;
06781                 }
06782             } else a001 = 0.0;
06783
06784             if (a100 < xarray[IJK(i,j,k)]) xarray[IJK(i,j,k)] = a100;
06785             if (a010 < yarray[IJK(i,j,k)]) yarray[IJK(i,j,k)] = a010;
06786             if (a001 < zarray[IJK(i,j,k)]) zarray[IJK(i,j,k)] = a001;
06787
06788             } /* k loop */
06789         } /* j loop */
06790     } /* i loop */
06791 }
06792
06793 /*
06794
06795     NOTE: This is the original version of the markSphere function. It's in here

```

```

06796 for reference and in case a reversion to the original code is needed.
06797 D. Gohara (2/14/08)
06798 */
06799 /*
06800 VPRIVATE void markSphere(
06801     double rtot, double *tpos,
06802     int nx, int ny, int nz,
06803     double hx, double hy, double hzed,
06804     double xmin, double ymin, double zmin,
06805     double *array, double markVal) {
06806
06807     int i, j, k, imin, imax, jmin, jmax, kmin, kmax;
06808     double dx, dx2, dy, dy2, dz, dz2;
06809     double rtot2, pos[3];
06810
06811     // Convert to grid reference frame
06812     pos[0] = tpos[0] - xmin;
06813     pos[1] = tpos[1] - ymin;
06814     pos[2] = tpos[2] - zmin;
06815
06816     rtot2 = VSQR(rtot);
06817
06818     dx = rtot + 0.5*hx;
06819     imin = VMAX2(0, (int)ceil((pos[0] - dx)/hx));
06820     imax = VMIN2(nx-1, (int)floor((pos[0] + dx)/hx));
06821     for (i=imin; i<=imax; i++) {
06822         dx2 = VSQR(pos[0] - hx*i);
06823         if (rtot2 > dx2) {
06824             dy = VSQRT(rtot2 - dx2) + 0.5*hy;
06825         } else {
06826             dy = 0.5*hy;
06827         }
06828         jmin = VMAX2(0, (int)ceil((pos[1] - dy)/hy));
06829         jmax = VMIN2(ny-1, (int)floor((pos[1] + dy)/hy));
06830         for (j=jmin; j<=jmax; j++) {
06831             dy2 = VSQR(pos[1] - hy*j);
06832             if (rtot2 > (dx2+dy2)) {
06833                 dz = VSQRT(rtot2-dx2-dy2)+0.5*hzed;
06834             } else {
06835                 dz = 0.5*hzed;
06836             }
06837             kmin = VMAX2(0, (int)ceil((pos[2] - dz)/hzed));
06838             kmax = VMIN2(nz-1, (int)floor((pos[2] + dz)/hzed));
06839             for (k=kmin; k<=kmax; k++) {
06840                 dz2 = VSQR(k*hzed - pos[2]);
06841                 if ((dz2 + dy2 + dx2) <= rtot2) {
06842                     array[IJK(i,j,k)] = markVal;
06843                 }
06844             } // k loop
06845         } // j loop
06846     } // i loop
06847 }
06848 */
06849 VPRIVATE void markSphere(double rtot, double *tpos,
06850     int nx, int ny, int nz,
06851     double hx, double hy, double hz,
06852     double xmin, double ymin, double zmin,
06853     double *array, double markVal) {
06854
06855     int i, j, k;
06856     double fi, fj, fk;
06857     int imin, imax;
06858     int jmin, jmax;
06859     int kmin, kmax;
06860     double dx2, dy2, dz2;
06861     double xrange, yrange, zrange;
06862     double rtot2, posx, posy, posz;
06863
06864     /* Convert to grid reference frame */
06865     posx = tpos[0] - xmin;
06866     posy = tpos[1] - ymin;
06867     posz = tpos[2] - zmin;
06868
06869     rtot2 = VSQR(rtot);
06870
06871     xrange = rtot + 0.5 * hx;
06872     yrange = rtot + 0.5 * hy;
06873     zrange = rtot + 0.5 * hz;
06874
06875     imin = VMAX2(0, (int)ceil((posx - xrange)/hx));
06876     jmin = VMAX2(0, (int)ceil((posy - yrange)/hy));

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```

06877     kmin = VMAX2(0, (int)ceil((posz - zrange)/hz));
06878
06879     imax = VMIN2(nx-1, (int)floor((posx + xrange)/hx));
06880     jmax = VMIN2(ny-1, (int)floor((posy + yrange)/hy));
06881     kmax = VMIN2(nz-1, (int)floor((posz + zrange)/hz));
06882
06883     for (i=imin,fi=imin; i<=imax; i++, fi+=1.) {
06884         dx2 = VSQR(posx - hx*fi);
06885         for (j=jmin,fj=jmin; j<=jmax; j++, fj+=1.) {
06886             dy2 = VSQR(posy - hy*fj);
06887             if((dx2 + dy2) > rtot2) continue;
06888             for (k=kmin, fk=kmin; k<=kmax; k++, fk+=1.) {
06889                 dz2 = VSQR(posz - hz*fk);
06890                 if ((dz2 + dy2 + dx2) <= rtot2) {
06891                     array[IJK(i,j,k)] = markVal;
06892                 }
06893             }
06894         }
06895     }
06896 }
06897
06898 VPRIVATE void zlapSolve(
06899     Vpmg *thee,
06900     double **solution,
06901     double **source,
06902     double **work1
06903 ) {
06904
06905     /* NOTE: this is an incredibly inefficient algorithm. The next
06906      * improvement is to focus on only non-zero entries in the source term.
06907      * The best improvement is to use a fast sine transform */
06908
06909     int n, nx, ny, nz, i, j, k, kx, ky, kz;
06910     double hx, hy, hzed, wx, wy, wz, xlen, ylen, zlen;
06911     double phix, phixpl, phixml, phiy, phiyml, phiypl, phiz, phizml, phizpl;
06912     double norm, coef, proj, eigx, eigy, eigz;
06913     double ihx2, ihy2, ihzed2;
06914     double *u, *f, *phi;
06915
06916     /* Snarf grid parameters */
06917     nx = thee->pmgp->nx;
06918     ny = thee->pmgp->ny;
06919     nz = thee->pmgp->nz;
06920     n = nx*ny*nz;
06921     hx = thee->pmgp->hx;
06922     ihx2 = 1.0/hx/hx;
06923     hy = thee->pmgp->hy;
06924     ihy2 = 1.0/hy/hy;
06925     hzed = thee->pmgp->hzed;
06926     ihzed2 = 1.0/hzed/hzed;
06927     xlen = thee->pmgp->xlen;
06928     ylen = thee->pmgp->ylen;
06929     zlen = thee->pmgp->zlen;
06930
06931     /* Set solution and source array pointers */
06932     u = *solution;
06933     f = *source;
06934     phi = *work1;
06935
06936     /* Zero out the solution vector */
06937     for (i=0; i<n; i++) thee->u[i] = 0.0;
06938
06939     /* Iterate through the wavenumbers */
06940     for (kx=1; kx<(nx-1); kx++) {
06941         wx = (VPI*(double)kx)/((double)nx - 1.0);
06942         eigx = 2.0*ihx2*(1.0 - cos(wx));
06943
06944         for (ky=1; ky<(ny-1); ky++) {
06945             wy = (VPI*(double)ky)/((double)ny - 1.0);
06946             eigy = 2.0*ihy2*(1.0 - cos(wy));
06947
06948             for (kz=1; kz<(nz-1); kz++) {
06949                 wz = (VPI*(double)kz)/((double)nz - 1.0);
06950                 eigz = 2.0*ihzed2*(1.0 - cos(wz));
06951
06952                 /* Calculate the basis function.
06953                  * We could calculate each basis function as
06954                  *   phix(i) = sin(wx*i)
06955                  */
06956             }
06957         }
06958     }

```

```

06958      *   phiy(j) = sin(wy*j)
06959      *   phiz(k) = sin(wz*k)
06960      * However, this is likely to be very expensive.
06961      * Therefore, we can use the fact that
06962      *   phix(i+1) = (2-hx*hx*eigx)*phix(i) - phix(i-1)
06963      * */
06964      for (i=1; i<(nx-1); i++) {
06965          if (i == 1) {
06966              phix = sin(wx*(double)i);
06967              phixml = 0.0;
06968          } else {
06969              phixpl = (2.0-hx*hx*eigx)*phix - phixml;
06970              phixml = phix;
06971              phix = phixpl;
06972          }
06973          /* phix = sin(wx*(double)i); */
06974          for (j=1; j<(ny-1); j++) {
06975              if (j == 1) {
06976                  phiy = sin(wy*(double)j);
06977                  phiyml = 0.0;
06978              } else {
06979                  phiypl = (2.0-hy*hy*eigy)*phiy - phiyml;
06980                  phiyml = phiy;
06981                  phiy = phiypl;
06982              }
06983              /* phiy = sin(wy*(double)j); */
06984              for (k=1; k<(nz-1); k++) {
06985                  if (k == 1) {
06986                      phiz = sin(wz*(double)k);
06987                      phizml = 0.0;
06988                  } else {
06989                      phizpl = (2.0-hzed*hzed*eigz)*phiz - phizml;
06990                      phizml = phiz;
06991                      phiz = phizpl;
06992                  }
06993                  /* phiz = sin(wz*(double)k); */
06994                  phi[IJK(i,j,k)] = phix*phiy*phiz;
06995              }
06996          }
06997      }
06998  }
06999
07000
07001      /* Calculate the projection of the source function on this
07002      * basis function */
07003      proj = 0.0;
07004      for (i=1; i<(nx-1); i++) {
07005          for (j=1; j<(ny-1); j++) {
07006              for (k=1; k<(nz-1); k++) {
07007
07008                  proj += f[IJK(i,j,k)]*phi[IJK(i,j,k)];
07009
07010              } /* k loop */
07011          } /* j loop */
07012      } /* i loop */
07013
07014      /* Assemble the coefficient to weight the contribution of this
07015      * basis function to the solution */
07016      /* The first contribution is the projection */
07017      coef = proj;
07018      /* The second contribution is the eigenvalue */
07019      coef = coef/(eigx + eigy + eigz);
07020      /* The third contribution is the normalization factor */
07021      coef = (8.0/xlen/ylen/zlen)*coef;
07022      /* The fourth contribution is from scaling the diagonal */
07023      /* coef = hx*hy*hzed*coef; */
07024
07025      /* Evaluate the basis function at each grid point */
07026      for (i=1; i<(nx-1); i++) {
07027          for (j=1; j<(ny-1); j++) {
07028              for (k=1; k<(nz-1); k++) {
07029
07030                  u[IJK(i,j,k)] += coef*phi[IJK(i,j,k)];
07031
07032              } /* k loop */
07033          } /* j loop */
07034      } /* i loop */
07035
07036      } /* kz loop */
07037      } /* ky loop */
07038      } /* kx loop */

```

```

07039
07040 }
07041
07042 VPUBLIC int Vpmg_solveLaplace(Vpmg *thee) {
07043
07044     int i, j, k, ijk, nx, ny, nz, n, dilo, dihi, djlo, djhi, dklo, dkhi;
07045     double hx, hy, hzed, epsw, iepsw, scal, scalx, scaly, scalz;
07046
07047     nx = thee->pmgp->nx;
07048     ny = thee->pmgp->ny;
07049     nz = thee->pmgp->nz;
07050     n = nx*ny*nz;
07051     hx = thee->pmgp->hx;
07052     hy = thee->pmgp->hy;
07053     hzed = thee->pmgp->hzed;
07054     epsw = Vpbe_getSolventDiel(thee->pbe);
07055     iepsw = 1.0/epsw;
07056     scal = hx*hy*hzed;
07057     scalx = hx*hy/hzed;
07058     scaly = hx*hzed/hy;
07059     scalz = hx*hy/hzed;
07060
07061     if (!(thee->filled)) {
07062         Vnm_print(2, "Vpmg_solve: Need to call Vpmg_fillco()\n");
07063         return 0;
07064     }
07065
07066     /* Load boundary conditions into the RHS array */
07067     for (i=1; i<(nx-1); i++) {
07068
07069         if (i == 1) dilo = 1;
07070         else dilo = 0;
07071         if (i == nx-2) dihi = 1;
07072         else dihi = 0;
07073
07074         for (j=1; j<(ny-1); j++) {
07075
07076             if (j == 1) djlo = 1;
07077             else djlo = 0;
07078             if (j == ny-2) djhi = 1;
07079             else djhi = 0;
07080
07081             for (k=1; k<(nz-1); k++) {
07082
07083                 if (k == 1) dklo = 1;
07084                 else dklo = 0;
07085                 if (k == nz-2) dkhi = 1;
07086                 else dkhi = 0;
07087
07088                 thee->fcf[IJK(i,j,k)] = \
07089                     iepsw*scal*thee->charge[IJK(i,j,k)] \
07090                     + dilo*scalx*thee->gxcf[IJKx(j,k,0)] \
07091                     + dihi*scalx*thee->gxcf[IJKx(j,k,1)] \
07092                     + djlo*scaly*thee->gycf[IJKy(i,k,0)] \
07093                     + djhi*scaly*thee->gycf[IJKy(i,k,1)] \
07094                     + dklo*scalz*thee->gzcf[IJKz(i,j,0)] \
07095                     + dkhi*scalz*thee->gzcf[IJKz(i,j,1)] ;
07096
07097             }
07098         }
07099     }
07100
07101     /* Solve */
07102     zlapSolve( thee, &(thee->u), &(thee->fcf), &(thee->tcf) );
07103
07104     /* Add boundary conditions to solution */
07105     /* i faces */
07106     for (j=0; j<ny; j++) {
07107         for (k=0; k<nz; k++) {
07108             thee->u[IJK(0,j,k)] = thee->gxcf[IJKx(j,k,0)];
07109             thee->u[IJK(nx-1,j,k)] = thee->gxcf[IJKx(j,k,1)];
07110         }
07111     }
07112     /* j faces */
07113     for (i=0; i<nx; i++) {
07114         for (k=0; k<nz; k++) {
07115             thee->u[IJK(i,0,k)] = thee->gycf[IJKy(i,k,0)];
07116             thee->u[IJK(i,ny-1,k)] = thee->gycf[IJKy(i,k,1)];
07117         }
07118     }
07119     /* k faces */
07120

```

```

07121     for (i=0; i<nx; i++) {
07122         for (j=0; j<ny; j++) {
07123             thee->u[IJK(i,j,0)] = thee->gzcfc[IJKz(i,j,0)];
07124             thee->u[IJK(i,j,nz-1)] = thee->gzcfc[IJKz(i,j,1)];
07125         }
07126     }
07127
07128     return 1;
07129
07130 }
07131
07132 VPRIVATE double VFCHI4(int i, double f) {
07133     return (2.5+((double) (i)-(f)));
07134 }
07135
07136 VPRIVATE double bspline4(double x) {
07137     double m, m2;
07138     static double one6 = 1.0/6.0;
07139     static double one8 = 1.0/8.0;
07140     static double one24 = 1.0/24.0;
07141     static double thirteen24 = 13.0/24.0;
07142     static double fortyseven24 = 47.0/24.0;
07143     static double seventeen24 = 17.0/24.0;
07144
07145     if ((x > 0.0) && (x <= 1.0)){
07146         m = x*x;
07147         return one24*m*m;
07148     } else if ((x > 1.0) && (x <= 2.0)){
07149         m = x - 1.0;
07150         m2 = m*m;
07151         return -one8 + one6*x + m2*(0.25 + one6*m - one6*m2);
07152     } else if ((x > 2.0) && (x <= 3.0)){
07153         m = x - 2.0;
07154         m2 = m*m;
07155         return -thirteen24 + 0.5*x + m2*(-0.25 - 0.5*m + 0.25*m2);
07156     } else if ((x > 3.0) && (x <= 4.0)){
07157         m = x - 3.0;
07158         m2 = m*m;
07159         return fortyseven24 - 0.5*x + m2*(-0.25 + 0.5*m - one6*m2);
07160     } else if ((x > 4.0) && (x <= 5.0)){
07161         m = x - 4.0;
07162         m2 = m*m;
07163         return seventeen24 - one6*x + m2*(0.25 - one6*m + one24*m2);
07164     } else {
07165         return 0.0;
07166     }
07167 }
07168 }
07169
07170 VPUBLIC double dbspline4(double x) {
07171     double m, m2;
07172     static double one6 = 1.0/6.0;
07173     static double one3 = 1.0/3.0;
07174     static double two3 = 2.0/3.0;
07175     static double thirteen6 = 13.0/6.0;
07176
07177     if ((x > 0.0) && (x <= 1.0)){
07178         m2 = x*x;
07179         return one6*x*m2;
07180     } else if ((x > 1.0) && (x <= 2.0)){
07181         m = x - 1.0;
07182         m2 = m*m;
07183         return -one3 + 0.5*x + m2*(0.5 - two3*m);
07184     } else if ((x > 2.0) && (x <= 3.0)){
07185         m = x - 2.0;
07186         m2 = m*m;
07187         return 1.5 - 0.5*x + m2*(-1.5 + m);
07188     } else if ((x > 3.0) && (x <= 4.0)){
07189         m = x - 3.0;
07190         m2 = m*m;
07191         return 1.0 - 0.5*x + m2*(1.5 - two3*m);
07192     } else if ((x > 4.0) && (x <= 5.0)){
07193         m = x - 4.0;
07194         m2 = m*m;
07195         return -thirteen6 + 0.5*x + m2*(-0.5 + one6*m);
07196     } else {
07197         return 0.0;
07198     }
07199 }
07200 }
07201

```

```

07202 VPUBLIC double d2bspline4(double x) {
07203     double m, m2;
07204
07205     if ((x > 0.0) && (x <= 1.0)){
07206         return 0.5*x*x;
07207     } else if ((x > 1.0) && (x <= 2.0)){
07208         m = x - 1.0;
07209         m2 = m*m;
07210         return -0.5 + x - 2.0*m2;
07211     } else if ((x > 2.0) && (x <= 3.0)){
07212         m = x - 2.0;
07213         m2 = m*m;
07214         return 5.5 - 3.0*x + 3.0*m2;
07215     } else if ((x > 3.0) && (x <= 4.0)){
07216         m = x - 3.0;
07217         m2 = m*m;
07218         return -9.5 + 3.0*x - 2.0*m2;
07219     } else if ((x > 4.0) && (x <= 5.0)){
07220         m = x - 4.0;
07221         m2 = m*m;
07222         return 4.5 - x + 0.5*m2;
07223     } else {
07224         return 0.0;
07225     }
07226 }
07227 }
07228
07229 VPUBLIC double d3bspline4(double x) {
07230     if ((x > 0.0) && (x <= 1.0)) return x;
07231     else if ((x > 1.0) && (x <= 2.0)) return 5.0 - 4.0 * x;
07232     else if ((x > 2.0) && (x <= 3.0)) return -15.0 + 6.0 * x;
07233     else if ((x > 3.0) && (x <= 4.0)) return 15.0 - 4.0 * x;
07234     else if ((x > 4.0) && (x <= 5.0)) return x - 5.0;
07235     else return 0.0;
07236 }
07237 }
07238 }
07239
07240 VPUBLIC void fillcoPermanentMultipole(Vpmg *thee) {
07241     Valist *alist;
07242     Vpbe *pbe;
07243     Vatom *atom;
07244     /* Conversions */
07245     double zmagic, f;
07246     /* Grid */
07247     double xmin, xmax, ymin, ymax, zmin, zmax;
07248     double xlen, ylen, zlen, position[3], ifloat, jfloat, kfloat;
07249     double hx, hy, hzed, *apos;
07250     /* Multipole */
07251     double charge, *dipole, *quad;
07252     double c, ux, uy, uz, qxx, qyx, qyy, qzx, qzy, qzz, qave;
07253     /* B-spline weights */
07254     double mx, my, mz, dmx, dmy, dmz, d2mx, d2my, d2mz;
07255     double mi, mj, mk;
07256     /* Loop variables */
07257     int i, ii, jj, kk, nx, ny, nz, iatom;
07258     int im2, im1, ip1, ip2, jm2, jm1, jp1, jp2, km2, km1, kp1, kp2;
07259
07260     /* sanity check */
07261     double mir, mjr, mkr, mr2;
07262     double debye, mc, mux, muy, muz, mqxx, mqyx, mqyy, mqzx, mqzy, mqzz;
07263
07264     VASSERT(thee != VNULL);
07265
07266     /* Get PBE info */
07267     pbe = thee->pbe;
07268     alist = pbe->alist;
07269     zmagic = Vpbe_getZmagic(pbe);
07270
07271     /* Mesh info */
07272     nx = thee->pmgp->nx;
07273     ny = thee->pmgp->ny;
07274     nz = thee->pmgp->nz;
07275     hx = thee->pmgp->hx;
07276     hy = thee->pmgp->hy;
07277     hzed = thee->pmgp->hzed;
07278
07279     /* Conversion */
07280     f = zmagic/(hx*hy*hzed);
07281
07282

```

```

07283      /* Define the total domain size */
07284      xlen = thee->pmgp->xlen;
07285      ylen = thee->pmgp->ylen;
07286      zlen = thee->pmgp->zlen;
07287
07288      /* Define the min/max dimensions */
07289      xmin = thee->pmgp->xcent - (xlen/2.0);
07290      ymin = thee->pmgp->ycent - (ylen/2.0);
07291      zmin = thee->pmgp->zcent - (zlen/2.0);
07292      xmax = thee->pmgp->xcent + (xlen/2.0);
07293      ymax = thee->pmgp->ycent + (ylen/2.0);
07294      zmax = thee->pmgp->zcent + (zlen/2.0);
07295
07296      /* Fill in the source term (permanent atomic multipoles) */
07297      Vnm_print(0, "fillcoPermanentMultipole: filling in source term.\n");
07298      for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
07299
07300          atom = Valist_getAtom(alist, iatom);
07301          apos = Vatom_getPosition(atom);
07302
07303          c = Vatom_getCharge(atom)*f;
07304
07305          #if defined(WITH_TINKER)
07306              dipole = Vatom_getDipole(atom);
07307              ux = dipole[0]/hx*f;
07308              uy = dipole[1]/hy*f;
07309              uz = dipole[2]/hz*f;
07310              quad = Vatom_getQuadrupole(atom);
07311              qxx = (1.0/3.0)*quad[0]/(hx*hx)*f;
07312              qyx = (2.0/3.0)*quad[3]/(hx*hy)*f;
07313              qyy = (1.0/3.0)*quad[4]/(hy*hy)*f;
07314              qzx = (2.0/3.0)*quad[6]/(hz*hx)*f;
07315              qzy = (2.0/3.0)*quad[7]/(hz*hy)*f;
07316              qzz = (1.0/3.0)*quad[8]/(hz*hz)*f;
07317          #else
07318              ux = 0.0;
07319              uy = 0.0;
07320              uz = 0.0;
07321              qxx = 0.0;
07322              qyx = 0.0;
07323              qyy = 0.0;
07324              qzx = 0.0;
07325              qzy = 0.0;
07326              qzz = 0.0;
07327          #endif /* if defined(WITH_TINKER) */
07328
07329          /* check
07330          mc = 0.0;
07331          mux = 0.0;
07332          muy = 0.0;
07333          muz = 0.0;
07334          mqxx = 0.0;
07335          mqyx = 0.0;
07336          mqyy = 0.0;
07337          mqzx = 0.0;
07338          mqzy = 0.0;
07339          mqzz = 0.0; */
07340
07341          /* Make sure we're on the grid */
07342          if ((apos[0]<=(xmin-2*hx)) || (apos[0]>=(xmax+2*hx)) || \
07343              (apos[1]<=(ymin-2*hy)) || (apos[1]>=(ymax+2*hy)) || \
07344              (apos[2]<=(zmin-2*hz)) || (apos[2]>=(zmax+2*hz))) {
07345              Vnm_print(2, "fillcoPermanentMultipole: Atom #%d at (%4.3f, %4.3f, %4.3f) is off the mesh
(ignoreing this atom):\n", iatom, apos[0], apos[1], apos[2]);
07346              Vnm_print(2, "fillcoPermanentMultipole: xmin = %g, xmax = %g\n", xmin, xmax);
07347              Vnm_print(2, "fillcoPermanentMultipole: ymin = %g, ymax = %g\n", ymin, ymax);
07348              Vnm_print(2, "fillcoPermanentMultipole: zmin = %g, zmax = %g\n", zmin, zmax);
07349              fflush(stderr);
07350          } else {
07351
07352              /* Convert the atom position to grid reference frame */
07353              position[0] = apos[0] - xmin;
07354              position[1] = apos[1] - ymin;
07355              position[2] = apos[2] - zmin;
07356
07357              /* Figure out which vertices we're next to */
07358              ifloat = position[0]/hx;
07359              jfloat = position[1]/hy;
07360              kfloat = position[2]/hz;
07361
07362              ip1 = (int)ceil(ifloat);

```



```

07363         ip2 = ip1 + 2;
07364         im1 = (int)floor(iffloat);
07365         im2 = im1 - 2;
07366         jp1 = (int)ceil(jffloat);
07367         jp2 = jp1 + 2;
07368         jm1 = (int)floor(jffloat);
07369         jm2 = jm1 - 2;
07370         kp1 = (int)ceil(kffloat);
07371         kp2 = kp1 + 2;
07372         km1 = (int)floor(kffloat);
07373         km2 = km1 - 2;
07374
07375         /* This step shouldn't be necessary, but it saves nasty debugging
07376          * later on if something goes wrong */
07377         ip2 = VMIN2(ip2,nx-1);
07378         ip1 = VMIN2(ip1,nx-1);
07379         im1 = VMAX2(im1,0);
07380         im2 = VMAX2(im2,0);
07381         jp2 = VMIN2(jp2,ny-1);
07382         jp1 = VMIN2(jp1,ny-1);
07383         jm1 = VMAX2(jm1,0);
07384         jm2 = VMAX2(jm2,0);
07385         kp2 = VMIN2(kp2,nz-1);
07386         kp1 = VMIN2(kp1,nz-1);
07387         km1 = VMAX2(km1,0);
07388         km2 = VMAX2(km2,0);
07389
07390         /* Now assign fractions of the charge to the nearby verts */
07391         for (ii=im2; ii<=ip2; ii++) {
07392             mi = VFCHI4(ii,iffloat);
07393             mx = bspline4(mi);
07394             dmx = dbspline4(mi);
07395             d2mx = d2bspline4(mi);
07396             for (jj=jm2; jj<=jp2; jj++) {
07397                 mj = VFCHI4(jj,jffloat);
07398                 my = bspline4(mj);
07399                 dmy = dbspline4(mj);
07400                 d2my = d2bspline4(mj);
07401                 for (kk=km2; kk<=kp2; kk++) {
07402                     mk = VFCHI4(kk,kffloat);
07403                     mz = bspline4(mk);
07404                     dmz = dbspline4(mk);
07405                     d2mz = d2bspline4(mk);
07406                     charge = mx*my*mz*c -
07407                             dmx*my*mz*ux - mx*dmy*mz*uy - mx*my*dmz*uz +
07408                             d2mx*my*mz*qxx +
07409                             dmx*dmy*mz*qyx + mx*d2my*mz*qyy +
07410                             dmx*my*dmz*qzx + mx*dmy*dmz*qzy + mx*my*d2mz*qzz;
07411                     three->charge[IJK(ii,jj,kk)] += charge;
07412
07413                     /* sanity check - recalculate traceless multipoles
07414                      from the grid charge distribution for this
07415                      site.
07416
07417                     mir = (mi - 2.5) * hx;
07418                     mjr = (mj - 2.5) * hy;
07419                     mkr = (mk - 2.5) * hzed;
07420                     mr2 = mir*mir+mjr*mjr+mkr*mkr;
07421                     mc += charge;
07422                     mux += mir * charge;
07423                     muy += mjr * charge;
07424                     muz += mkr * charge;
07425                     mqxx += (1.5*mir*mir - 0.5*mr2) * charge;
07426                     mqyx += 1.5*mjr*mir * charge;
07427                     mqyy += (1.5*mjr*mjr - 0.5*mr2) * charge;
07428                     mqzx += 1.5*mkr*mir * charge;
07429                     mqzy += 1.5*mkr*mjr * charge;
07430                     mqzz += (1.5*mkr*mkr - 0.5*mr2) * charge;
07431                     */
07432                 }
07433             }
07434         }
07435     } /* endif (on the mesh) */
07436
07437     /* print out the Grid vs. Ideal Point Multipole. */
07438
07439     /*
07440     debye = 4.8033324;
07441     mc = mc/f;
07442     mux = mux/f*debye;
07443     muy = muy/f*debye;

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07444     muz = muz/f*debye;
07445     mqxx = mqxx/f*debye;
07446     mqyy = mqyy/f*debye;
07447     mqzz = mqzz/f*debye;
07448     mqyx = mqyx/f*debye;
07449     mqzx = mqzx/f*debye;
07450     mqzy = mqzy/f*debye;
07451
07452     printf(" Grid v. Actual Permanent Multipole for Site %i\n",iatom);
07453     printf(" G: %10.6f\n",mc);
07454     printf(" A: %10.6f\n\n",c/f);
07455     printf(" G: %10.6f %10.6f %10.6f\n",mux,muy,muz);
07456     printf(" A: %10.6f %10.6f %10.6f\n\n",
07457           (ux * hx / f) * debye,
07458           (uy * hy / f) * debye,
07459           (uz * hzed /f) * debye);
07460     printf(" G: %10.6f\n",mqxx);
07461     printf(" A: %10.6f\n",quad[0]*debye);
07462     printf(" G: %10.6f %10.6f\n",mqyx,mqyy);
07463     printf(" A: %10.6f %10.6f\n",quad[3]*debye,quad[4]*debye);
07464     printf(" G: %10.6f %10.6f %10.6f\n",mqzx,mqzy,mqzz);
07465     printf(" A: %10.6f %10.6f %10.6f\n\n",
07466           quad[6]*debye,quad[7]*debye,quad[8]*debye); */
07467
07468 } /* endfor (each atom) */
07469 }
07470
07471 #if defined(WITH_TINKER)
07472
07473 VPUBLIC void fillcoInducedDipole(Vpmg *thee) {
07474
07475     Valist *alist;
07476     Vpbe *pbe;
07477     Vatom *atom;
07478     /* Conversions */
07479     double zmagic, f;
07480     /* Grid */
07481     double xmin, xmax, ymin, ymax, zmin, zmax;
07482     double xlen, ylen, zlen, ifloat, jfloat, kfloat;
07483     double hx, hy, hzed, *apos, position[3];
07484     /* B-spline weights */
07485     double mx, my, mz, dmx, dmy, dmz;
07486     /* Dipole */
07487     double charge, *dipole, ux,uy,uz;
07488     double mi,mj,mk;
07489     /* Loop indeces */
07490     int i, ii, jj, kk, nx, ny, nz, iatom;
07491     int im2, im1, ip1, ip2, jm2, jm1, jpl, jp2, km2, km1, kp1, kp2;
07492
07493     double debye;
07494     double mux,muy,muz;
07495     double mir,mjr,mkr;
07496
07497     VASSERT(thee != VNULL);
07498
07499     /* Get PBE info */
07500     pbe = thee->pbe;
07501     alist = pbe->alist;
07502     zmagic = Vpbe_getZmagic(pbe);
07503
07504     /* Mesh info */
07505     nx = thee->pmgp->nx;
07506     ny = thee->pmgp->ny;
07507     nz = thee->pmgp->nz;
07508     hx = thee->pmgp->hx;
07509     hy = thee->pmgp->hy;
07510     hzed = thee->pmgp->hzed;
07511
07512     /* Conversion */
07513     f = zmagic/(hx*hy*hzed);
07514
07515     /* Define the total domain size */
07516     xlen = thee->pmgp->xlen;
07517     ylen = thee->pmgp->ylen;
07518     zlen = thee->pmgp->zlen;
07519
07520     /* Define the min/max dimensions */
07521     xmin = thee->pmgp->xcent - (xlen/2.0);
07522     ymin = thee->pmgp->ycent - (ylen/2.0);
07523     zmin = thee->pmgp->zcent - (zlen/2.0);
07524     xmax = thee->pmgp->xcent + (xlen/2.0);

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```

07525     ymax = thee->pmpg->ycent + (ylen/2.0);
07526     zmax = thee->pmpg->zcent + (zlen/2.0);
07527
07528     /* Fill in the source term (induced dipoles) */
07529     Vnm_print(0, "fillcoInducedDipole: filling in the source term.\n");
07530     for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
07531
07532         atom = Valist_getAtom(alist, iatom);
07533         apos = Vatom_getPosition(atom);
07534
07535         dipole = Vatom_getInducedDipole(atom);
07536         ux = dipole[0]/hx*f;
07537         uy = dipole[1]/hy*f;
07538         uz = dipole[2]/hz*f;
07539
07540         mux = 0.0;
07541         muy = 0.0;
07542         muz = 0.0;
07543
07544         /* Make sure we're on the grid */
07545         if ((apos[0]<=(xmin-2*hx)) || (apos[0]>=(xmax+2*hx)) || \
07546             (apos[1]<=(ymin-2*hy)) || (apos[1]>=(ymax+2*hy)) || \
07547             (apos[2]<=(zmin-2*hz)) || (apos[2]>=(zmax+2*hz))) {
07548             Vnm_print(2, "fillcoInducedDipole: Atom #d at (%4.3f, %4.3f, %4.3f) is off the mesh (ignoring
this atom):\n", iatom, apos[0], apos[1], apos[2]);
07549             Vnm_print(2, "fillcoInducedDipole: xmin = %g, xmax = %g\n", xmin, xmax);
07550             Vnm_print(2, "fillcoInducedDipole: ymin = %g, ymax = %g\n", ymin, ymax);
07551             Vnm_print(2, "fillcoInducedDipole: zmin = %g, zmax = %g\n", zmin, zmax);
07552             fflush(stderr);
07553         } else {
07554
07555             /* Convert the atom position to grid reference frame */
07556             position[0] = apos[0] - xmin;
07557             position[1] = apos[1] - ymin;
07558             position[2] = apos[2] - zmin;
07559
07560             /* Figure out which vertices we're next to */
07561             ifloat = position[0]/hx;
07562             jfloat = position[1]/hy;
07563             kfloat = position[2]/hz;
07564
07565             ip1 = (int)ceil(ifloat);
07566             ip2 = ip1 + 2;
07567             im1 = (int)floor(ifloat);
07568             im2 = im1 - 2;
07569             jp1 = (int)ceil(jfloat);
07570             jp2 = jp1 + 2;
07571             jm1 = (int)floor(jfloat);
07572             jm2 = jm1 - 2;
07573             kp1 = (int)ceil(kfloat);
07574             kp2 = kp1 + 2;
07575             km1 = (int)floor(kfloat);
07576             km2 = km1 - 2;
07577
07578             /* This step shouldn't be necessary, but it saves nasty debugging
* later on if something goes wrong */
07579             ip2 = VMIN2(ip2,nx-1);
07580             ip1 = VMIN2(ip1,nx-1);
07581             im1 = VMAX2(im1,0);
07582             im2 = VMAX2(im2,0);
07583             jp2 = VMIN2(jp2,ny-1);
07584             jp1 = VMIN2(jp1,ny-1);
07585             jm1 = VMAX2(jm1,0);
07586             jm2 = VMAX2(jm2,0);
07587             kp2 = VMIN2(kp2,nz-1);
07588             kp1 = VMIN2(kp1,nz-1);
07589             km1 = VMAX2(km1,0);
07590             km2 = VMAX2(km2,0);
07591
07592             /* Now assign fractions of the dipole to the nearby verts */
07593             for (ii=im2; ii<=ip2; ii++) {
07594                 mi = VFCHI4(ii,ifloat);
07595                 mx = bspline4(mi);
07596                 dmX = dbspline4(mi);
07597                 for (jj=jm2; jj<=jp2; jj++) {
07598                     mj = VFCHI4(jj,jfloat);
07599                     my = bspline4(mj);
07600                     dmy = dbspline4(mj);
07601                     for (kk=km2; kk<=kp2; kk++) {
07602                         mk = VFCHI4(kk,kfloat);
07603                         mz = bspline4(mk);

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07605         dmz = dbspline4(mk);
07606         charge = -dmx*my*mz*ux - mx*dmy*mz*uy - mx*my*dmz*uz;
07607         thee->charge[IJK(ii,jj,kk)] += charge;
07608
07609         /*
07610         mir = (mi - 2.5) * hx;
07611         mjr = (mj - 2.5) * hy;
07612         mkr = (mk - 2.5) * hzed;
07613         mux += mir * charge;
07614         muy += mjr * charge;
07615         muz += mkr * charge;
07616         */
07617     }
07618 }
07619 }
07620 } /* endif (on the mesh) */
07621
07622 /* check
07623 debye = 4.8033324;
07624 mux = mux/f*debye;
07625 muy = muy/f*debye;
07626 muz = muz/f*debye;
07627
07628 printf(" Grid v. Actual Induced Dipole for Site %i\n",iatom);
07629 printf(" G: %10.6f %10.6f %10.6f\n",mux,muy,muz);
07630 printf(" A: %10.6f %10.6f %10.6f\n",
07631         (ux * hx / f) * debye,
07632         (uy * hy / f) * debye,
07633         (uz * hzed /f) * debye);
07634 */
07635 } /* endfor (each atom) */
07636 }
07637 }
07638
07639 VPUBLIC void fillcoNLInducedDipole(Vpmpg *thee) {
07640
07641     Valist *alist;
07642     Vpbe *pbe;
07643     Vatom *atom;
07644     /* Conversions */
07645     double zmagic, f;
07646     /* Grid */
07647     double xmin, xmax, ymin, ymax, zmin, zmax;
07648     double xlen, ylen, zlen, ifloat, jfloat, kfloat;
07649     double hx, hy, hzed, *apos, position[3];
07650     /* B-spline weights */
07651     double mx, my, mz, dmx, dmy, dmz;
07652     /* Dipole */
07653     double charge, *dipole, ux,uy,uz;
07654     double mi,mj,mk;
07655     /* Loop indeces */
07656     int i, ii, jj, kk, nx, ny, nz, iatom;
07657     int im2, im1, ip1, ip2, jm2, jm1, jp1, jp2, km2, km1, kp1, kp2;
07658
07659     /* sanity check
07660     double debye;
07661     double mux,muy,muz;
07662     double mir,mjr,mkr;
07663     */
07664
07665     VASSERT(thee != VNULL);
07666
07667     /* Get PBE info */
07668     pbe = thee->pbe;
07669     alist = pbe->alist;
07670     zmagic = Vpbe_getZmagic(pbe);
07671
07672     /* Mesh info */
07673     nx = thee->pmgp->nx;
07674     ny = thee->pmgp->ny;
07675     nz = thee->pmgp->nz;
07676     hx = thee->pmgp->hx;
07677     hy = thee->pmgp->hy;
07678     hzed = thee->pmgp->hzed;
07679
07680     /* Conversion */
07681     f = zmagic/(hx*hy*hzed);
07682
07683     /* Define the total domain size */
07684     xlen = thee->pmgp->xlen;
07685     ylen = thee->pmgp->ylen;

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07686     zlen = thee->pmgp->zlen;
07687
07688     /* Define the min/max dimensions */
07689     xmin = thee->pmgp->xcent - (xlen/2.0);
07690     ymin = thee->pmgp->ycent - (ylen/2.0);
07691     zmin = thee->pmgp->zcent - (zlen/2.0);
07692     xmax = thee->pmgp->xcent + (xlen/2.0);
07693     ymax = thee->pmgp->ycent + (ylen/2.0);
07694     zmax = thee->pmgp->zcent + (zlen/2.0);
07695
07696     /* Fill in the source term (non-local induced dipoles) */
07697     Vnm_print(0, "fillcoNLInducedDipole: filling in source term.\n");
07698     for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
07699
07700         atom = Valist_getAtom(alist, iatom);
07701         apos = Vatom_getPosition(atom);
07702
07703         dipole = Vatom_getNLInducedDipole(atom);
07704         ux = dipole[0]/hx*f;
07705         uy = dipole[1]/hy*f;
07706         uz = dipole[2]/hz*f;
07707
07708         /*
07709         mux = 0.0;
07710         muy = 0.0;
07711         muz = 0.0;
07712         */
07713
07714         /* Make sure we're on the grid */
07715         if ((apos[0]<=(xmin-2*hx)) || (apos[0]>=(xmax+2*hx)) || \
07716             (apos[1]<=(ymin-2*hy)) || (apos[1]>=(ymax+2*hy)) || \
07717             (apos[2]<=(zmin-2*hz)) || (apos[2]>=(zmax+2*hz))) {
07718             Vnm_print(2, "fillcoNLInducedDipole: Atom #d at (%4.3f, %4.3f,%4.3f) is off the mesh
07719 (ignoring this atom):\n", iatom, apos[0], apos[1], apos[2]);
07719             Vnm_print(2, "fillcoNLInducedDipole: xmin = %g, xmax = %g\n", xmin, xmax);
07720             Vnm_print(2, "fillcoNLInducedDipole: ymin = %g, ymax = %g\n", ymin, ymax);
07721             Vnm_print(2, "fillcoNLInducedDipole: zmin = %g, zmax = %g\n", zmin, zmax);
07722             fflush(stderr);
07723         } else {
07724
07725             /* Convert the atom position to grid reference frame */
07726             position[0] = apos[0] - xmin;
07727             position[1] = apos[1] - ymin;
07728             position[2] = apos[2] - zmin;
07729
07730             /* Figure out which vertices we're next to */
07731             ifloat = position[0]/hx;
07732             jfloat = position[1]/hy;
07733             kfloat = position[2]/hz;
07734
07735             ip1 = (int)ceil(ifloat);
07736             ip2 = ip1 + 2;
07737             im1 = (int)floor(ifloat);
07738             im2 = im1 - 2;
07739             jp1 = (int)ceil(jfloat);
07740             jp2 = jp1 + 2;
07741             jm1 = (int)floor(jfloat);
07742             jm2 = jm1 - 2;
07743             kp1 = (int)ceil(kfloat);
07744             kp2 = kp1 + 2;
07745             km1 = (int)floor(kfloat);
07746             km2 = km1 - 2;
07747
07748             /* This step shouldn't be necessary, but it saves nasty debugging
07749              * later on if something goes wrong */
07750             ip2 = VMIN2(ip2,nx-1);
07751             ip1 = VMIN2(ip1,nx-1);
07752             im1 = VMAX2(im1,0);
07753             im2 = VMAX2(im2,0);
07754             jp2 = VMIN2(jp2,ny-1);
07755             jp1 = VMIN2(jp1,ny-1);
07756             jm1 = VMAX2(jm1,0);
07757             jm2 = VMAX2(jm2,0);
07758             kp2 = VMIN2(kp2,nz-1);
07759             kp1 = VMIN2(kp1,nz-1);
07760             km1 = VMAX2(km1,0);
07761             km2 = VMAX2(km2,0);
07762
07763             /* Now assign fractions of the non local induced dipole
07764              to the nearby verts */
07765             for (ii=im2; ii<=ip2; ii++) {

```

```

07766         mi = VFCHI4(ii,ifloat);
07767         mx = bspline4(mi);
07768         dmx = dbspline4(mi);
07769         for (jj=jm2; jj<=jp2; jj++) {
07770             mj = VFCHI4(jj,jfloat);
07771             my = bspline4(mj);
07772             dmy = dbspline4(mj);
07773             for (kk=km2; kk<=kp2; kk++) {
07774                 mk = VFCHI4(kk,kfloat);
07775                 mz = bspline4(mk);
07776                 dmz = dbspline4(mk);
07777                 charge = -dmx*my*mz*ux - mx*dmy*mz*uy - mx*my*dmz*uz;
07778                 thee->charge[IJK(ii,jj,kk)] += charge;
07779
07780                 /*
07781                 mir = (mi - 2.5) * hx;
07782                 mjr = (mj - 2.5) * hy;
07783                 mkr = (mk - 2.5) * hzed;
07784                 mux += mir * charge;
07785                 muy += mjr * charge;
07786                 muz += mkr * charge;
07787                 */
07788             }
07789         }
07790     } /* endif (on the mesh) */
07791 }
07792
07793 /*
07794 debye = 4.8033324;
07795 mux = mux/f*debye;
07796 muy = muy/f*debye;
07797 muz = muz/f*debye;
07798
07799 printf(" Grid v. Actual Non-Local Induced Dipole for Site %i\n",iatom);
07800 printf(" G: %10.6f %10.6f %10.6f\n",mux,muy,muz);
07801 printf(" A: %10.6f %10.6f %10.6f\n",
07802        (ux * hx / f) * debye,
07803        (uy * hy / f) * debye,
07804        (uz * hzed / f) * debye); */
07805 } /* endfor (each atom) */
07806 }
07807 }
07808
07809 VPUBLIC double Vpmg_qfPermanentMultipoleEnergy(Vpmg *thee, int atomID) {
07810
07811     double *u;
07812     Vatom *atom;
07813     /* Grid variables */
07814     int nx, ny, nz;
07815     double xmax, xmin, ymax, ymin, zmax, zmin;
07816     double hx, hy, hzed, ifloat, jfloat, kfloat;
07817     double mi, mj, mk;
07818     double *position;
07819     /* B-spline weights */
07820     double mx, my, mz, dmx, dmy, dmz, d2mx, d2my, d2mz;
07821     /* Loop indeces */
07822     int ip1,ip2,im1,im2,jp1,jp2,jm1,jm2,kp1,kp2,km1,km2;
07823     int i,j,ii,jj,kk;
07824     /* Potential, field, field gradient and multipole components */
07825     double pot, rfe[3], rfde[3][3], energy;
07826     double f, charge, *dipole, *quad;
07827     double qxx, qyx, qyy, qzx, qzy, qzz;
07828
07829     VASSERT(thee != VNULL);
07830     VASSERT(thee->filled);
07831
07832     /* Get the mesh information */
07833     nx = thee->pmgp->nx;
07834     ny = thee->pmgp->ny;
07835     nz = thee->pmgp->nz;
07836     hx = thee->pmgp->hx;
07837     hy = thee->pmgp->hy;
07838     hzed = thee->pmgp->hzed;
07839     xmax = thee->xf[nx-1];
07840     ymax = thee->yf[ny-1];
07841     zmax = thee->zf[nz-1];
07842     xmin = thee->xf[0];
07843     ymin = thee->yf[0];
07844     zmin = thee->zf[0];
07845
07846

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```

07847     u = thee->u;
07848
07849     atom = Valist_getAtom(thee->pbe->alist, atomID);
07850
07851     /* Currently all atoms must be in the same partition. */
07852
07853     VASSERT(atom->partID != 0);
07854
07855     /* Convert the atom position to grid coordinates */
07856
07857     position = Vatom_getPosition(atom);
07858     ifloat = (position[0] - xmin)/hx;
07859     jfloat = (position[1] - ymin)/hy;
07860     kfloat = (position[2] - zmin)/hz;
07861     ip1 = (int)ceil(ifloat);
07862     ip2 = ip1 + 2;
07863     im1 = (int)floor(ifloat);
07864     im2 = im1 - 2;
07865     jp1 = (int)ceil(jfloat);
07866     jp2 = jp1 + 2;
07867     jm1 = (int)floor(jfloat);
07868     jm2 = jm1 - 2;
07869     kp1 = (int)ceil(kfloat);
07870     kp2 = kp1 + 2;
07871     km1 = (int)floor(kfloat);
07872     km2 = km1 - 2;
07873
07874     /* This step shouldn't be necessary, but it saves nasty debugging
07875      * later on if something goes wrong */
07876     ip2 = VMIN2(ip2, nx-1);
07877     ip1 = VMIN2(ip1, nx-1);
07878     im1 = VMAX2(im1, 0);
07879     im2 = VMAX2(im2, 0);
07880     jp2 = VMIN2(jp2, ny-1);
07881     jp1 = VMIN2(jp1, ny-1);
07882     jm1 = VMAX2(jm1, 0);
07883     jm2 = VMAX2(jm2, 0);
07884     kp2 = VMIN2(kp2, nz-1);
07885     kp1 = VMIN2(kp1, nz-1);
07886     km1 = VMAX2(km1, 0);
07887     km2 = VMAX2(km2, 0);
07888
07889     /* Initialize observables to zero */
07890     energy = 0.0;
07891     pot = 0.0;
07892     for (i=0; i<3; i++) {
07893         rfe[i] = 0.0;
07894         for (j=0; j<3; j++) {
07895             rfde[i][j] = 0.0;
07896         }
07897     }
07898
07899     for (ii=im2; ii<=ip2; ii++) {
07900         mi = VFCHI4(ii, ifloat);
07901         mx = bspline4(mi);
07902         dm1 = db spline4(mi);
07903         d2mx = d2bspline4(mi);
07904         for (jj=jm2; jj<=jp2; jj++) {
07905             mj = VFCHI4(jj, jfloat);
07906             my = bspline4(mj);
07907             dmy = db spline4(mj);
07908             d2my = d2bspline4(mj);
07909             for (kk=km2; kk<=kp2; kk++) {
07910                 mk = VFCHI4(kk, kfloat);
07911                 mz = bspline4(mk);
07912                 dmz = db spline4(mk);
07913                 d2mz = d2bspline4(mk);
07914                 f = u[IJK(ii, jj, kk)];
07915                 /* potential */
07916                 pot += f*mx*my*mz;
07917                 /* field */
07918                 rfe[0] += f*dm1*my*mz/hx;
07919                 rfe[1] += f*mx*dmy*mz/hy;
07920                 rfe[2] += f*mx*my*dmz/hz;
07921                 /* field gradient */
07922                 rfde[0][0] += f*d2mx*my*mz/(hx*hx);
07923                 rfde[1][0] += f*dm1*dmy*mz/(hy*hx);
07924                 rfde[1][1] += f*mx*d2my*mz/(hy*hy);
07925                 rfde[2][0] += f*dm1*my*dmz/(hx*hz);
07926                 rfde[2][1] += f*mx*dmy*dmz/(hy*hz);
07927                 rfde[2][2] += f*mx*my*d2mz/(hz*hz);

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07928     }
07929     }
07930 }
07931
07932 charge = Vatom_getCharge(atom);
07933 dipole = Vatom_getDipole(atom);
07934 quad = Vatom_getQuadrupole(atom);
07935 qxx = quad[0]/3.0;
07936 qyx = quad[3]/3.0;
07937 qyy = quad[4]/3.0;
07938 qzx = quad[6]/3.0;
07939 qzy = quad[7]/3.0;
07940 qzz = quad[8]/3.0;
07941
07942 energy = pot * charge
07943         - rfe[0] * dipole[0]
07944         - rfe[1] * dipole[1]
07945         - rfe[2] * dipole[2]
07946         + rfde[0][0]*qxx
07947         + 2.0*rfde[1][0]*qyx + rfde[1][1]*qyy
07948         + 2.0*rfde[2][0]*qzx + 2.0*rfde[2][1]*qzy + rfde[2][2]*qzz;
07949
07950 return energy;
07951 }
07952
07953 VPUBLIC void Vpmg_fieldSpline4(Vpmg *thee, int atomID, double field[3]) {
07954
07955     Vatom *atom;
07956     double *u, f;
07957     /* Grid variables */
07958     int nx, ny, nz;
07959     double xmax, xmin, ymax, ymin, zmax, zmin;
07960     double hx, hy, hzed, ifloat, jfloat, kfloat;
07961     double *apos, position[3];
07962     /* B-Spline weights */
07963     double mx, my, mz, dmx, dmy, dmz;
07964     double mi, mj, mk;
07965     /* Loop indeces */
07966     int ip1, ip2, im1, im2, jp1, jp2, jm1, jm2, kp1, kp2, km1, km2;
07967     int i, j, ii, jj, kk;
07968
07969
07970     VASSERT (thee != VNULL);
07971
07972     /* Get the mesh information */
07973     nx = thee->pmgp->nx;
07974     ny = thee->pmgp->ny;
07975     nz = thee->pmgp->nz;
07976     hx = thee->pmgp->hx;
07977     hy = thee->pmgp->hy;
07978     hzed = thee->pmgp->hzed;
07979     xmax = thee->xf[nx-1];
07980     ymax = thee->yf[ny-1];
07981     zmax = thee->zf[nz-1];
07982     xmin = thee->xf[0];
07983     ymin = thee->yf[0];
07984     zmin = thee->zf[0];
07985
07986     u = thee->u;
07987
07988     atom = Valist_getAtom(thee->pbe->alist, atomID);
07989
07990     /* Currently all atoms must be in the same partition. */
07991
07992     VASSERT (atom->partID != 0);
07993
07994     /* Convert the atom position to grid coordinates */
07995
07996     apos = Vatom_getPosition(atom);
07997     position[0] = apos[0] - xmin;
07998     position[1] = apos[1] - ymin;
07999     position[2] = apos[2] - zmin;
08000     ifloat = position[0]/hx;
08001     jfloat = position[1]/hy;
08002     kfloat = position[2]/hzed;
08003     ip1 = (int)ceil(ifloat);
08004     ip2 = ip1 + 2;
08005     im1 = (int)floor(ifloat);
08006     im2 = im1 - 2;
08007     jp1 = (int)ceil(jfloat);
08008     jp2 = jp1 + 2;

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08009     jml = (int)floor(jfloat);
08010     jm2 = jml - 2;
08011     kpl = (int)ceil(kfloat);
08012     kp2 = kpl + 2;
08013     kml = (int)floor(kfloat);
08014     km2 = kml - 2;
08015
08016     /* This step shouldn't be necessary, but it saves nasty debugging
08017      * later on if something goes wrong */
08018     ip2 = VMIN2(ip2,nx-1);
08019     ip1 = VMIN2(ip1,nx-1);
08020     im1 = VMAX2(im1,0);
08021     im2 = VMAX2(im2,0);
08022     jp2 = VMIN2(jp2,ny-1);
08023     jp1 = VMIN2(jp1,ny-1);
08024     jml = VMAX2(jml,0);
08025     jm2 = VMAX2(jm2,0);
08026     kp2 = VMIN2(kp2,nz-1);
08027     kpl = VMIN2(kpl,nz-1);
08028     kml = VMAX2(kml,0);
08029     km2 = VMAX2(km2,0);
08030
08031     for (i=0;i<3;i++){
08032         field[i] = 0.0;
08033     }
08034
08035     for (ii=im2; ii<=ip2; ii++) {
08036         mi = VFCHI4(ii,ifloat);
08037         mx = bspline4(mi);
08038         dmx = dbspline4(mi);
08039         for (jj=jm2; jj<=jp2; jj++) {
08040             mj = VFCHI4(jj,jfloat);
08041             my = bspline4(mj);
08042             dmy = dbspline4(mj);
08043             for (kk=km2; kk<=kp2; kk++) {
08044                 mk = VFCHI4(kk,kfloat);
08045                 mz = bspline4(mk);
08046                 dmz = dbspline4(mk);
08047                 f = u[IJK(ii,jj,kk)];
08048
08049                 field[0] += f*dmx*my*mz/hx;
08050                 field[1] += f*mx*dmy*mz/hy;
08051                 field[2] += f*mx*my*dmz/hzed;
08052             }
08053         }
08054     }
08055 }
08056
08057 VPUBLIC void Vpmg_qfPermanentMultipoleForce(Vpmg *thee, int atomID,
08058                                             double force[3], double torque[3]) {
08059
08060     Vatom *atom;
08061     double f, *u, *apos, position[3];
08062
08063     /* Grid variables */
08064     int nx,ny,nz;
08065     double xlen, ylen, zlen, xmin, ymin, zmin, xmax, ymax, zmax;
08066     double hx, hy, hzed, ifloat, jfloat, kfloat;
08067
08068     /* B-spline weights */
08069     double mx, my, mz, dmx, dmy, dmz, d2mx, d2my, d2mz, d3mx, d3my, d3mz;
08070     double mi, mj, mk;
08071
08072     /* Loop indeces */
08073     int i, j, k, ii, jj, kk;
08074     int im2, im1, ip1, ip2, jm2, jml, jp1, jp2, km2, kml, kpl, kp2;
08075
08076     /* Potential, field, field gradient and 2nd field gradient */
08077     double pot, e[3], de[3][3], d2e[3][3][3];
08078
08079     /* Permanent multipole components */
08080     double *dipole, *quad;
08081     double c, ux, uy, uz, qxx, qxy, qxz, qyx, qyy, qyz, qzx, qzy, qzz;
08082
08083     VASSERT(thee != VNULL);
08084     VASSERT(thee->filled);
08085
08086     atom = Valist_getAtom(thee->pbe->alist, atomID);
08087
08088     /* Currently all atoms must be in the same partition. */
08089

```

```

08090     VASSERT(atom->partID != 0);
08091
08092     apos = Vatom_getPosition(atom);
08093
08094     c = Vatom_getCharge(atom);
08095     dipole = Vatom_getDipole(atom);
08096     ux = dipole[0];
08097     uy = dipole[1];
08098     uz = dipole[2];
08099     quad = Vatom_getQuadrupole(atom);
08100     qxx = quad[0]/3.0;
08101     qxy = quad[1]/3.0;
08102     qxz = quad[2]/3.0;
08103     qyx = quad[3]/3.0;
08104     qyy = quad[4]/3.0;
08105     qyz = quad[5]/3.0;
08106     qzx = quad[6]/3.0;
08107     qzy = quad[7]/3.0;
08108     qzz = quad[8]/3.0;
08109
08110     /* Initialize observables */
08111     pot = 0.0;
08112     for (i=0; i<3; i++){
08113         e[i] = 0.0;
08114         for (j=0; j<3; j++){
08115             de[i][j] = 0.0;
08116             for (k=0; k<3; k++){
08117                 d2e[i][j][k] = 0.0;
08118             }
08119         }
08120     }
08121
08122     /* Mesh info */
08123     nx = thee->pmgpp->nx;
08124     ny = thee->pmgpp->ny;
08125     nz = thee->pmgpp->nz;
08126     hx = thee->pmgpp->hx;
08127     hy = thee->pmgpp->hy;
08128     hzed = thee->pmgpp->hzed;
08129     xlen = thee->pmgpp->xlen;
08130     ylen = thee->pmgpp->ylen;
08131     zlen = thee->pmgpp->zlen;
08132     xmin = thee->pmgpp->xmin;
08133     ymin = thee->pmgpp->ymin;
08134     zmin = thee->pmgpp->zmin;
08135     xmax = thee->pmgpp->xmax;
08136     ymax = thee->pmgpp->ymax;
08137     zmax = thee->pmgpp->zmax;
08138     u = thee->u;
08139
08140     /* Make sure we're on the grid */
08141     if ((apos[0]<=(xmin+2*hx)) || (apos[0]>=(xmax-2*hx)) \
08142         || (apos[1]<=(ymin+2*hy)) || (apos[1]>=(ymax-2*hy)) \
08143         || (apos[2]<=(zmin+2*hzed)) || (apos[2]>=(zmax-2*hzed))) {
08144         Vnm_print(2, "qfPermanentMultipoleForce: Atom off the mesh (ignoring) %6.3f %6.3f %6.3f\n",
08145             apos[0], apos[1], apos[2]);
08146         fflush(stderr);
08147     } else {
08148         /* Convert the atom position to grid coordinates */
08149         position[0] = apos[0] - xmin;
08150         position[1] = apos[1] - ymin;
08151         position[2] = apos[2] - zmin;
08152         ifloat = position[0]/hx;
08153         jfloat = position[1]/hy;
08154         kfloat = position[2]/hzed;
08155         ip1 = (int)ceil(ifloat);
08156         ip2 = ip1 + 2;
08157         im1 = (int)floor(ifloat);
08158         im2 = im1 - 2;
08159         jp1 = (int)ceil(jfloat);
08160         jp2 = jp1 + 2;
08161         jm1 = (int)floor(jfloat);
08162         jm2 = jm1 - 2;
08163         kp1 = (int)ceil(kfloat);
08164         kp2 = kp1 + 2;
08165         km1 = (int)floor(kfloat);
08166         km2 = km1 - 2;
08167
08168         /* This step shouldn't be necessary, but it saves nasty debugging
08169          * later on if something goes wrong */

```

```

08170      ip2 = VMIN2(ip2,nx-1);
08171      ip1 = VMIN2(ip1,nx-1);
08172      im1 = VMAX2(im1,0);
08173      im2 = VMAX2(im2,0);
08174      jp2 = VMIN2(jp2,ny-1);
08175      jp1 = VMIN2(jp1,ny-1);
08176      jm1 = VMAX2(jm1,0);
08177      jm2 = VMAX2(jm2,0);
08178      kp2 = VMIN2(kp2,nz-1);
08179      kp1 = VMIN2(kp1,nz-1);
08180      km1 = VMAX2(km1,0);
08181      km2 = VMAX2(km2,0);
08182
08183      for (ii=im2; ii<=ip2; ii++) {
08184          mi = VFCHI4(ii,ifloat);
08185          mx = bspline4(mi);
08186          dmx = dbspline4(mi);
08187          d2mx = d2bspline4(mi);
08188          d3mx = d3bspline4(mi);
08189          for (jj=jm2; jj<=jp2; jj++) {
08190              mj = VFCHI4(jj,jfloat);
08191              my = bspline4(mj);
08192              dmy = dbspline4(mj);
08193              d2my = d2bspline4(mj);
08194              d3my = d3bspline4(mj);
08195              for (kk=km2; kk<=kp2; kk++) {
08196                  mk = VFCHI4(kk,kfloat);
08197                  mz = bspline4(mk);
08198                  dmz = dbspline4(mk);
08199                  d2mz = d2bspline4(mk);
08200                  d3mz = d3bspline4(mk);
08201                  f = u[IJK(ii,jj,kk)];
08202                  /* Potential */
08203                  pot += f*mx*my*mz;
08204                  /* Field */
08205                  e[0] += f*dmx*my*mz/hx;
08206                  e[1] += f*mx*dmy*mz/hy;
08207                  e[2] += f*mx*my*dmz/hzed;
08208                  /* Field gradient */
08209                  de[0][0] += f*d2mx*my*mz/(hx*hx);
08210                  de[1][0] += f*dmx*dmy*mz/(hy*hx);
08211                  de[1][1] += f*mx*d2my*mz/(hy*hy);
08212                  de[2][0] += f*dmx*my*dmz/(hx*hzed);
08213                  de[2][1] += f*mx*dmy*dmz/(hy*hzed);
08214                  de[2][2] += f*mx*my*d2mz/(hzed*hzed);
08215                  /* 2nd Field Gradient
08216                     VxVxVa */
08217                  d2e[0][0][0] += f*d3mx*my*mz/(hx*hx*hx);
08218                  d2e[0][0][1] += f*d2mx*dmy*mz/(hx*hy*hx);
08219                  d2e[0][0][2] += f*d2mx*my*dmz/(hx*hx*hzed);
08220                  /* VyVxVa */
08221                  d2e[1][0][0] += f*d2mx*dmy*mz/(hx*hx*hy);
08222                  d2e[1][0][1] += f*dmx*d2my*mz/(hx*hy*hy);
08223                  d2e[1][0][2] += f*dmx*dmy*dmz/(hx*hy*hzed);
08224                  /* VyVyVa */
08225                  d2e[1][1][0] += f*dmx*d2my*mz/(hx*hy*hy);
08226                  d2e[1][1][1] += f*mx*d3my*mz/(hy*hy*hy);
08227                  d2e[1][1][2] += f*mx*d2my*dmz/(hy*hy*hzed);
08228                  /* VzVxVa */
08229                  d2e[2][0][0] += f*d2mx*my*dmz/(hx*hx*hzed);
08230                  d2e[2][0][1] += f*dmx*dmy*dmz/(hx*hy*hzed);
08231                  d2e[2][0][2] += f*dmx*my*d2mz/(hx*hzed*hzed);
08232                  /* VzVyVa */
08233                  d2e[2][1][0] += f*dmx*dmy*dmz/(hx*hy*hzed);
08234                  d2e[2][1][1] += f*mx*d2my*dmz/(hy*hy*hzed);
08235                  d2e[2][1][2] += f*mx*dmy*d2mz/(hy*hzed*hzed);
08236                  /* VzVzVa */
08237                  d2e[2][2][0] += f*dmx*my*d2mz/(hx*hzed*hzed);
08238                  d2e[2][2][1] += f*mx*dmy*d2mz/(hy*hzed*hzed);
08239                  d2e[2][2][2] += f*mx*my*d3mz/(hzed*hzed*hzed);
08240              }
08241          }
08242      }
08243  }
08244
08245  /* Monopole Force */
08246  force[0] = e[0]*c;
08247  force[1] = e[1]*c;
08248  force[2] = e[2]*c;
08249
08250  /* Dipole Force */

```

```

08251     force[0] -= de[0][0]*ux+de[1][0]*uy+de[2][0]*uz;
08252     force[1] -= de[1][0]*ux+de[1][1]*uy+de[2][1]*uz;
08253     force[2] -= de[2][0]*ux+de[2][1]*uy+de[2][2]*uz;
08254
08255     /* Quadrupole Force */
08256     force[0] += d2e[0][0][0]*qxx
08257               + d2e[1][0][0]*qyx*2.0+d2e[1][1][0]*qyy
08258               + d2e[2][0][0]*qzx*2.0+d2e[2][1][0]*qzy*2.0+d2e[2][2][0]*qzz;
08259     force[1] += d2e[0][0][1]*qxx
08260               + d2e[1][0][1]*qyx*2.0+d2e[1][1][1]*qyy
08261               + d2e[2][0][1]*qzx*2.0+d2e[2][1][1]*qzy*2.0+d2e[2][2][1]*qzz;
08262     force[2] += d2e[0][0][2]*qxx
08263               + d2e[1][0][2]*qyx*2.0+d2e[1][1][2]*qyy
08264               + d2e[2][0][2]*qzx*2.0+d2e[2][1][2]*qzy*2.0+d2e[2][2][2]*qzz;
08265
08266     /* Dipole Torque */
08267     torque[0] = uy * e[2] - uz * e[1];
08268     torque[1] = uz * e[0] - ux * e[2];
08269     torque[2] = ux * e[1] - uy * e[0];
08270     /* Quadrupole Torque */
08271     de[0][1] = de[1][0];
08272     de[0][2] = de[2][0];
08273     de[1][2] = de[2][1];
08274     torque[0] -= 2.0*(qyx*de[0][2] + qyy*de[1][2] + qyz*de[2][2]
08275                  - qzx*de[0][1] - qzy*de[1][1] - qzz*de[2][1]);
08276     torque[1] -= 2.0*(qzx*de[0][0] + qzy*de[1][0] + qzz*de[2][0]
08277                  - qxx*de[0][2] - qxy*de[1][2] - qxz*de[2][2]);
08278     torque[2] -= 2.0*(qxx*de[0][1] + qxy*de[1][1] + qxz*de[2][1]
08279                  - qyx*de[0][0] - qyy*de[1][0] - qyz*de[2][0]);
08280
08281     /* printf(" qPhi Force %f %f %f\n", force[0], force[1], force[2]);
08282     printf(" qPhi Torque %f %f %f\n", torque[0], torque[1], torque[2]); */
08284 }
08285
08286 VPUBLIC void Vpmg_ibPermanentMultipoleForce(Vpmg *thee, int atomID,
08287                                             double force[3]) {
08288
08289     Valist *alist;
08290     Vacc *acc;
08291     Vpbe *pbe;
08292     Vatom *atom;
08293     Vsurf_Meth srfm;
08294
08295     /* Grid variables */
08296     double *apos, position[3], arad, irad, zkappa2, hx, hy, hzed;
08297     double xlen, ylen, zlen, xmin, ymin, zmin, xmax, ymax, zmax, rtot2;
08298     double rtot, dx, dx2, dy, dy2, dz, dz2, gpos[3], tgrad[3], fmag;
08299     double izmagic;
08300     int i, j, k, nx, ny, nz, imin, imax, jmin, jmax, kmin, kmax;
08301
08302     VASSERT(thee != VNULL);
08303
08304     /* Nonlinear PBE is not implemented for AMOEBA */
08305     VASSERT(!thee->pmgp->nonlin);
08306
08307     acc = thee->pbe->acc;
08308     srfm = thee->surfMeth;
08309     atom = Valist_getAtom(thee->pbe->alist, atomID);
08310
08311     /* Currently all atoms must be in the same partition. */
08312
08313     VASSERT(atom->partID != 0);
08314     apos = Vatom_getPosition(atom);
08315     arad = Vatom_getRadius(atom);
08316
08317     /* Reset force */
08318     force[0] = 0.0;
08319     force[1] = 0.0;
08320     force[2] = 0.0;
08321
08322     /* Get PBE info */
08323     pbe = thee->pbe;
08324     acc = pbe->acc;
08325     alist = pbe->alist;
08326     irad = Vpbe_getMaxIonRadius(pbe);
08327     zkappa2 = Vpbe_getZkappa2(pbe);
08328     izmagic = 1.0/Vpbe_getZmagic(pbe);
08329
08330     /* Should be a check for this further up. */
08331     VASSERT(zkappa2 > VPMGSMALL);

```

```

08332
08333     /* Mesh info */
08334     nx = thee->pmgp->nx;
08335     ny = thee->pmgp->ny;
08336     nz = thee->pmgp->nz;
08337     hx = thee->pmgp->hx;
08338     hy = thee->pmgp->hy;
08339     hzed = thee->pmgp->hz;
08340     xlen = thee->pmgp->xlen;
08341     ylen = thee->pmgp->ylen;
08342     zlen = thee->pmgp->zlen;
08343     xmin = thee->pmgp->xmin;
08344     ymin = thee->pmgp->ymin;
08345     zmin = thee->pmgp->zmin;
08346     xmax = thee->pmgp->xmax;
08347     ymax = thee->pmgp->ymax;
08348     zmax = thee->pmgp->zmax;
08349
08350     /* Make sure we're on the grid */
08351     if ((apos[0]<=xmin) || (apos[0]>=xmax) || \
08352         (apos[1]<=ymin) || (apos[1]>=ymax) || \
08353         (apos[2]<=zmin) || (apos[2]>=zmax)) {
08354         Vnm_print(2, "ibPermanentMultipoleForce: Atom %d at (%4.3f, %4.3f, %4.3f) is off the mesh
08355         (ignoring):\n", atomID, apos[0], apos[1], apos[2]);
08356         Vnm_print(2, "ibPermanentMultipoleForce:  xmin = %g, xmax = %g\n", xmin, xmax);
08357         Vnm_print(2, "ibPermanentMultipoleForce:  ymin = %g, ymax = %g\n", ymin, ymax);
08358         Vnm_print(2, "ibPermanentMultipoleForce:  zmin = %g, zmax = %g\n", zmin, zmax);
08359         fflush(stderr);
08360     } else {
08361         /* Convert the atom position to grid reference frame */
08362         position[0] = apos[0] - xmin;
08363         position[1] = apos[1] - ymin;
08364         position[2] = apos[2] - zmin;
08365
08366         /* Integrate over points within this atom's (inflated) radius */
08367         rtot = (irad + arad + thee->splineWin);
08368         rtot2 = VSQR(rtot);
08369         dx = rtot + 0.5*hx;
08370         imin = VMAX2(0, (int)ceil((position[0] - dx)/hx));
08371         imax = VMIN2(nx-1, (int)floor((position[0] + dx)/hx));
08372         for (i=imin; i<=imax; i++) {
08373             dx2 = VSQR(position[0] - hx*i);
08374             if (rtot2 > dx2) dy = VSQRT(rtot2 - dx2) + 0.5*hy;
08375             else dy = 0.5*hy;
08376             jmin = VMAX2(0, (int)ceil((position[1] - dy)/hy));
08377             jmax = VMIN2(ny-1, (int)floor((position[1] + dy)/hy));
08378             for (j=jmin; j<=jmax; j++) {
08379                 dy2 = VSQR(position[1] - hy*j);
08380                 if (rtot2 > (dx2+dy2)) dz = VSQRT(rtot2-dx2-dy2)+0.5*hz;
08381                 else dz = 0.5*hz;
08382                 kmin = VMAX2(0, (int)ceil((position[2] - dz)/hz));
08383                 kmax = VMIN2(nz-1, (int)floor((position[2] + dz)/hz));
08384                 for (k=kmin; k<=kmax; k++) {
08385                     dz2 = VSQR(k*hz - position[2]);
08386                     /* See if grid point is inside idvw radius and set ccf
08387                     * accordingly (do spline assignment here) */
08388                     if ((dz2 + dy2 + dx2) <= rtot2) {
08389                         gpos[0] = i*hx + xmin;
08390                         gpos[1] = j*hy + ymin;
08391                         gpos[2] = k*hz + zmin;
08392                         Vpmg_splineSelect(srfm, acc, gpos, thee->splineWin, irad, atom, tgrad);
08393                         fmag = VSQR(thee->u[IJK(i,j,k)]*thee->kappa[IJK(i,j,k)]);
08394                         force[0] += (zkappa2*fmag*tgrad[0]);
08395                         force[1] += (zkappa2*fmag*tgrad[1]);
08396                         force[2] += (zkappa2*fmag*tgrad[2]);
08397                     }
08398                 } /* k loop */
08399             } /* j loop */
08400         } /* i loop */
08401     }
08402
08403     force[0] = force[0] * 0.5 * hx * hy * hzed * izmagic;
08404     force[1] = force[1] * 0.5 * hx * hy * hzed * izmagic;
08405     force[2] = force[2] * 0.5 * hx * hy * hzed * izmagic;
08406
08407 }
08408
08409 VPUBLIC void Vpmg_dbPermanentMultipoleForce(Vpmg *thee, int atomID,
08410     double force[3]) {
08411

```

```

08412     Vpbe *acc;
08413     Vpbe *pbe;
08414     Vatom *atom;
08415     Vsurf_Meth srfrm;
08416
08417     double *apos, position[3], arad, hx, hy, hzed, izmagic, deps, depsi;
08418     double xlen, ylen, zlen, xmin, ymin, zmin, xmax, ymax, zmax, rtot2, epsp;
08419     double rtot, dx, gpos[3], tgrad[3], dbFmag, epsw, kT;
08420     double *u, Hxijk, Hyijk, Hzijk, Hximljk, Hyijmlk, Hzijkm1;
08421     double dHxijk[3], dHyijk[3], dHzijk[3], dHximljk[3], dHyijmlk[3];
08422     double dHzijkm1[3];
08423     int i, j, k, l, nx, ny, nz, imin, imax, jmin, jmax, kmin, kmax;
08424
08425     VASSERT(thee != VNULL);
08426
08427     acc = thee->pbe->acc;
08428     srfrm = thee->surfMeth;
08429     atom = Valist_getAtom(thee->pbe->alist, atomID);
08430
08431     /* Currently all atoms must be in the same partition. */
08432
08433     VASSERT(atom->partID != 0);
08434     arad = Vatom_getRadius(atom);
08435     apos = Vatom_getPosition(atom);
08436
08437     /* Reset force */
08438     force[0] = 0.0;
08439     force[1] = 0.0;
08440     force[2] = 0.0;
08441
08442     /* Get PBE info */
08443     pbe = thee->pbe;
08444     acc = pbe->acc;
08445     epsp = Vpbe_getSoluteDiel(pbe);
08446     epsw = Vpbe_getSolventDiel(pbe);
08447     kT = Vpbe_getTemperature(pbe) * (1e-3) * Vunit_Na * Vunit_kb;
08448     izmagic = 1.0 / Vpbe_getZmagic(pbe);
08449
08450
08451     deps = (epsw - epsp);
08452     depsi = 1.0 / deps;
08453
08454     VASSERT(VABS(deps) > VPMGSMALL);
08455
08456     /* Mesh info */
08457     nx = thee->pmgpp->nx;
08458     ny = thee->pmgpp->ny;
08459     nz = thee->pmgpp->nz;
08460     hx = thee->pmgpp->hx;
08461     hy = thee->pmgpp->hy;
08462     hzed = thee->pmgpp->hzed;
08463     xlen = thee->pmgpp->xlen;
08464     ylen = thee->pmgpp->ylen;
08465     zlen = thee->pmgpp->zlen;
08466     xmin = thee->pmgpp->xmin;
08467     ymin = thee->pmgpp->ymin;
08468     zmin = thee->pmgpp->zmin;
08469     xmax = thee->pmgpp->xmax;
08470     ymax = thee->pmgpp->ymax;
08471     zmax = thee->pmgpp->zmax;
08472     u = thee->u;
08473
08474     /* Make sure we're on the grid */
08475     if ((apos[0] <= xmin) || (apos[0] >= xmax) || \
08476         (apos[1] <= ymin) || (apos[1] >= ymax) || \
08477         (apos[2] <= zmin) || (apos[2] >= zmax)) {
08478         Vnm_print(2, "dbPermanentMultipoleForce: Atom at (%4.3f, %4.3f, %4.3f) is off the mesh
08479 (ignoring):\n", apos[0], apos[1], apos[2]);
08480         Vnm_print(2, "dbPermanentMultipoleForce: xmin = %g, xmax = %g\n", xmin, xmax);
08481         Vnm_print(2, "dbPermanentMultipoleForce: ymin = %g, ymax = %g\n", ymin, ymax);
08482         Vnm_print(2, "dbPermanentMultipoleForce: zmin = %g, zmax = %g\n", zmin, zmax);
08483         fflush(stderr);
08484     } else {
08485         /* Convert the atom position to grid reference frame */
08486         position[0] = apos[0] - xmin;
08487         position[1] = apos[1] - ymin;
08488         position[2] = apos[2] - zmin;
08489
08490         /* Integrate over points within this atom's (inflated) radius */
08491         rtot = (arad + thee->splineWin);

```

```

08492     rtot2 = VSQR(rtot);
08493     dx = rtot/hx;
08494     imin = (int)floor((position[0]-rtot)/hx);
08495     if (imin < 1) {
08496         Vnm_print(2, "dbPermanentMultipoleForce: Atom off grid!\n");
08497         return;
08498     }
08499     imax = (int)ceil((position[0]+rtot)/hx);
08500     if (imax > (nx-2)) {
08501         Vnm_print(2, "dbPermanentMultipoleForce: Atom off grid!\n");
08502         return;
08503     }
08504     jmin = (int)floor((position[1]-rtot)/hy);
08505     if (jmin < 1) {
08506         Vnm_print(2, "dbPermanentMultipoleForce: Atom off grid!\n");
08507         return;
08508     }
08509     jmax = (int)ceil((position[1]+rtot)/hy);
08510     if (jmax > (ny-2)) {
08511         Vnm_print(2, "dbPermanentMultipoleForce: Atom off grid!\n");
08512         return;
08513     }
08514     kmin = (int)floor((position[2]-rtot)/hz);
08515     if (kmin < 1) {
08516         Vnm_print(2, "dbPermanentMultipoleForce: Atom off grid!\n");
08517         return;
08518     }
08519     kmax = (int)ceil((position[2]+rtot)/hz);
08520     if (kmax > (nz-2)) {
08521         Vnm_print(2, "dbPermanentMultipoleForce: Atom off grid!\n");
08522         return;
08523     }
08524     for (i=imin; i<=imax; i++) {
08525         for (j=jmin; j<=jmax; j++) {
08526             for (k=kmin; k<=kmax; k++) {
08527                 /* i,j,k */
08528                 gpos[0] = (i+0.5)*hx + xmin;
08529                 gpos[1] = j*hy + ymin;
08530                 gpos[2] = k*hz + zmin;
08531                 Hxijk = (thee->epsx[IJK(i,j,k)] - epsp)*depsi;
08532                 Vpmg_splineSelect(srffm, acc, gpos, thee->splineWin, 0.,
08533                     atom, dHxijk);
08534                 for (l=0; l<3; l++) dHxijk[l] *= Hxijk;
08535                 gpos[0] = i*hx + xmin;
08536                 gpos[1] = (j+0.5)*hy + ymin;
08537                 gpos[2] = k*hz + zmin;
08538                 Hyijk = (thee->epsy[IJK(i,j,k)] - epsp)*depsi;
08539                 Vpmg_splineSelect(srffm, acc, gpos, thee->splineWin, 0.,
08540                     atom, dHyijk);
08541                 for (l=0; l<3; l++) dHyijk[l] *= Hyijk;
08542                 gpos[0] = i*hx + xmin;
08543                 gpos[1] = j*hy + ymin;
08544                 gpos[2] = (k+0.5)*hz + zmin;
08545                 Hzijk = (thee->epsz[IJK(i,j,k)] - epsp)*depsi;
08546                 Vpmg_splineSelect(srffm, acc, gpos, thee->splineWin, 0.,
08547                     atom, dHzijk);
08548                 for (l=0; l<3; l++) dHzijk[l] *= Hzijk;
08549                 /* i-1,j,k */
08550                 gpos[0] = (i-0.5)*hx + xmin;
08551                 gpos[1] = j*hy + ymin;
08552                 gpos[2] = k*hz + zmin;
08553                 Hximljk = (thee->epsx[IJK(i-1,j,k)] - epsp)*depsi;
08554                 Vpmg_splineSelect(srffm, acc, gpos, thee->splineWin, 0.,
08555                     atom, dHximljk);
08556                 for (l=0; l<3; l++) dHximljk[l] *= Hximljk;
08557                 /* i,j-1,k */
08558                 gpos[0] = i*hx + xmin;
08559                 gpos[1] = (j-0.5)*hy + ymin;
08560                 gpos[2] = k*hz + zmin;
08561                 Hyijmlk = (thee->epsy[IJK(i,j-1,k)] - epsp)*depsi;
08562                 Vpmg_splineSelect(srffm, acc, gpos, thee->splineWin, 0.,
08563                     atom, dHyijmlk);
08564                 for (l=0; l<3; l++) dHyijmlk[l] *= Hyijmlk;
08565                 /* i,j,k-1 */
08566                 gpos[0] = i*hx + xmin;
08567                 gpos[1] = j*hy + ymin;
08568                 gpos[2] = (k-0.5)*hz + zmin;
08569                 Hzijkml = (thee->epsz[IJK(i,j,k-1)] - epsp)*depsi;
08570                 Vpmg_splineSelect(srffm, acc, gpos, thee->splineWin, 0.,
08571                     atom, dHzijkml);
08572                 for (l=0; l<3; l++) dHzijkml[l] *= Hzijkml;

```

```

08573         dbFmag = u[IJK(i,j,k)];
08574         tgrad[0] =
08575             (dHxijk[0] * (u[IJK(i+1,j,k)]-u[IJK(i,j,k)])
08576             + dHximljk[0] * (u[IJK(i-1,j,k)]-u[IJK(i,j,k)])) /VSQR(hx)
08577             + (dHyijk[0] * (u[IJK(i,j+1,k)]-u[IJK(i,j,k)])
08578             + dHyijmlk[0] * (u[IJK(i,j-1,k)]-u[IJK(i,j,k)])) /VSQR(hy)
08579             + (dHzijk[0] * (u[IJK(i,j,k+1)]-u[IJK(i,j,k)])
08580             + dHzijkm1[0] * (u[IJK(i,j,k-1)]-u[IJK(i,j,k)])) /VSQR(hzed);
08581         tgrad[1] =
08582             (dHxijk[1] * (u[IJK(i+1,j,k)]-u[IJK(i,j,k)])
08583             + dHximljk[1] * (u[IJK(i-1,j,k)]-u[IJK(i,j,k)])) /VSQR(hx)
08584             + (dHyijk[1] * (u[IJK(i,j+1,k)]-u[IJK(i,j,k)])
08585             + dHyijmlk[1] * (u[IJK(i,j-1,k)]-u[IJK(i,j,k)])) /VSQR(hy)
08586             + (dHzijk[1] * (u[IJK(i,j,k+1)]-u[IJK(i,j,k)])
08587             + dHzijkm1[1] * (u[IJK(i,j,k-1)]-u[IJK(i,j,k)])) /VSQR(hzed);
08588         tgrad[2] =
08589             (dHxijk[2] * (u[IJK(i+1,j,k)]-u[IJK(i,j,k)])
08590             + dHximljk[2] * (u[IJK(i-1,j,k)]-u[IJK(i,j,k)])) /VSQR(hx)
08591             + (dHyijk[2] * (u[IJK(i,j+1,k)]-u[IJK(i,j,k)])
08592             + dHyijmlk[2] * (u[IJK(i,j-1,k)]-u[IJK(i,j,k)])) /VSQR(hy)
08593             + (dHzijk[2] * (u[IJK(i,j,k+1)]-u[IJK(i,j,k)])
08594             + dHzijkm1[2] * (u[IJK(i,j,k-1)]-u[IJK(i,j,k)])) /VSQR(hzed);
08595         force[0] += (dbFmag*tgrad[0]);
08596         force[1] += (dbFmag*tgrad[1]);
08597         force[2] += (dbFmag*tgrad[2]);
08598     } /* k loop */
08599 } /* j loop */
08600 } /* i loop */
08601 force[0] = -force[0]*hx*hy*hzed*deps*0.5*izmagic;
08602 force[1] = -force[1]*hx*hy*hzed*deps*0.5*izmagic;
08603 force[2] = -force[2]*hx*hy*hzed*deps*0.5*izmagic;
08604 }
08605 }
08606
08607 VPUBLIC void Vpmg_qfDirectPolForce(Vpmg *thee, Vgrid* perm, Vgrid *induced,
08608                                     int atomID, double force[3], double torque[3]) {
08609
08610     Vatom *atom;
08611     Vpbe *pbe;
08612     double f, fp, *u, *up, *apos, position[3];
08613
08614     /* Grid variables */
08615     int nx,ny,nz;
08616     double xlen, ylen, zlen, xmin, ymin, zmin, xmax, ymax, zmax;
08617     double hx, hy, hzed, ifloat, jfloat, kfloat;
08618
08619     /* B-spline weights */
08620     double mx, my, mz, dmxx, dmy, dmz, d2mx, d2my, d2mz, d3mx, d3my, d3mz;
08621     double mi, mj, mk;
08622
08623     /* Loop indeces */
08624     int i, j, k, ii, jj, kk;
08625     int im2, im1, ip1, ip2, jm2, jm1, jp1, jp2, km2, km1, kp1, kp2;
08626
08627     /* Permanent potential, field, field gradient and 2nd field gradient */
08628     double pot, e[3], de[3][3], d2e[3][3][3];
08629     /* Induced dipole field */
08630     double dep[3][3];
08631
08632     /* Permanent multipole components */
08633     double *dipole, *quad;
08634     double c, ux, uy, uz, qxx, qxy, qxz, qyx, qyy, qyz, qzx, qzy, qzz;
08635     double uix, uiy, uiz;
08636
08637     VASSERT(thee != VNULL);
08638     VASSERT(induced != VNULL); /* the potential due to permanent multipoles */
08639     VASSERT(induced != VNULL); /* the potential due to local induced dipoles */
08640     VASSERT(thee->pbe != VNULL);
08641     VASSERT(thee->pbe->alist != VNULL);
08642
08643     atom = Valist_getAtom(thee->pbe->alist, atomID);
08644     VASSERT(atom->partID != 0); /* all atoms must be in the same partition */
08645     apos = Vatom_getPosition(atom);
08646
08647     c = Vatom_getCharge(atom);
08648     dipole = Vatom_getDipole(atom);
08649     ux = dipole[0];
08650     uy = dipole[1];
08651     uz = dipole[2];
08652     quad = Vatom_getQuadrupole(atom);
08653     qxx = quad[0]/3.0;

```



```

08654     qxy = quad[1]/3.0;
08655     qxz = quad[2]/3.0;
08656     qyx = quad[3]/3.0;
08657     qyy = quad[4]/3.0;
08658     qyz = quad[5]/3.0;
08659     qzx = quad[6]/3.0;
08660     qzy = quad[7]/3.0;
08661     qzz = quad[8]/3.0;
08662
08663     dipole = Vatom_getInducedDipole(atom);
08664     uix = dipole[0];
08665     uiy = dipole[1];
08666     uiz = dipole[2];
08667
08668     /* Reset Field Gradients */
08669     pot = 0.0;
08670     for (i=0;i<3;i++){
08671         e[i] = 0.0;
08672         for (j=0;j<3;j++){
08673             de[i][j] = 0.0;
08674             dep[i][j] = 0.0;
08675             for (k=0;k<3;k++){
08676                 d2e[i][j][k] = 0.0;
08677             }
08678         }
08679     }
08680
08681     /* Mesh info */
08682     nx = thee->pmgp->nx;
08683     ny = thee->pmgp->ny;
08684     nz = thee->pmgp->nz;
08685     hx = thee->pmgp->hx;
08686     hy = thee->pmgp->hy;
08687     hzed = thee->pmgp->hzed;
08688     xlen = thee->pmgp->xlen;
08689     ylen = thee->pmgp->ylen;
08690     zlen = thee->pmgp->zlen;
08691     xmin = thee->pmgp->xmin;
08692     ymin = thee->pmgp->ymin;
08693     zmin = thee->pmgp->zmin;
08694     xmax = thee->pmgp->xmax;
08695     ymax = thee->pmgp->ymax;
08696     zmax = thee->pmgp->zmax;
08697     u = induced->data;
08698     up = perm->data;
08699
08700     /* Make sure we're on the grid */
08701     if ((apos[0]<=(xmin+2*hx)) || (apos[0]>=(xmax-2*hx)) \
08702         || (apos[1]<=(ymin+2*hy)) || (apos[1]>=(ymax-2*hy)) \
08703         || (apos[2]<=(zmin+2*hzed)) || (apos[2]>=(zmax-2*hzed))) {
08704         Vnm_print(2, "qfDirectPolForce: Atom off the mesh (ignoring) %6.3f %6.3f %6.3f\n", apos[0],
08705         apos[1], apos[2]);
08706         fflush(stderr);
08707     } else {
08708
08709         /* Convert the atom position to grid coordinates */
08710         position[0] = apos[0] - xmin;
08711         position[1] = apos[1] - ymin;
08712         position[2] = apos[2] - zmin;
08713         ifloat = position[0]/hx;
08714         jfloat = position[1]/hy;
08715         kfloat = position[2]/hzed;
08716         ip1 = (int)ceil(ifloat);
08717         ip2 = ip1 + 2;
08718         im1 = (int)floor(ifloat);
08719         im2 = im1 - 2;
08720         jp1 = (int)ceil(jfloat);
08721         jp2 = jp1 + 2;
08722         jm1 = (int)floor(jfloat);
08723         jm2 = jm1 - 2;
08724         kp1 = (int)ceil(kfloat);
08725         kp2 = kp1 + 2;
08726         km1 = (int)floor(kfloat);
08727         km2 = km1 - 2;
08728
08729         /* This step shouldn't be necessary, but it saves nasty debugging
08730          * later on if something goes wrong */
08731         ip2 = VMIN2(ip2,nx-1);
08732         ip1 = VMIN2(ip1,nx-1);
08733         im1 = VMAX2(im1,0);

```

```

08734     im2 = VMAX2(im2,0);
08735     jp2 = VMIN2(jp2,ny-1);
08736     jp1 = VMIN2(jp1,ny-1);
08737     jm1 = VMAX2(jm1,0);
08738     jm2 = VMAX2(jm2,0);
08739     kp2 = VMIN2(kp2,nz-1);
08740     kp1 = VMIN2(kp1,nz-1);
08741     km1 = VMAX2(km1,0);
08742     km2 = VMAX2(km2,0);
08743
08744     for (ii=im2; ii<=ip2; ii++) {
08745         mi = VFCHI4(ii,ifloat);
08746         mx = bspline4(mi);
08747         dmx = dbspline4(mi);
08748         d2mx = d2bspline4(mi);
08749         d3mx = d3bspline4(mi);
08750         for (jj=jm2; jj<=jp2; jj++) {
08751             mj = VFCHI4(jj,jfloat);
08752             my = bspline4(mj);
08753             dmy = dbspline4(mj);
08754             d2my = d2bspline4(mj);
08755             d3my = d3bspline4(mj);
08756             for (kk=km2; kk<=kp2; kk++) {
08757                 mk = VFCHI4(kk,kfloat);
08758                 mz = bspline4(mk);
08759                 dmz = dbspline4(mk);
08760                 d2mz = d2bspline4(mk);
08761                 d3mz = d3bspline4(mk);
08762                 f = u[IJK(ii,jj,kk)];
08763                 fp = up[IJK(ii,jj,kk)];
08764                 /* The potential */
08765                 pot += f*mx*my*mz;
08766                 /* The field */
08767                 e[0] += f*dmx*my*mz/hx;
08768                 e[1] += f*mx*dmy*mz/hy;
08769                 e[2] += f*mx*my*dmz/hzed;
08770                 /* The gradient of the field */
08771                 de[0][0] += f*d2mx*my*mz/(hx*hx);
08772                 de[1][0] += f*dmx*dmy*mz/(hy*hx);
08773                 de[1][1] += f*mx*d2my*mz/(hy*hy);
08774                 de[2][0] += f*dmx*my*dmz/(hx*hzed);
08775                 de[2][1] += f*mx*dmy*dmz/(hy*hzed);
08776                 de[2][2] += f*mx*my*d2mz/(hzed*hzed);
08777                 /* The gradient of the (permanent) field */
08778                 dep[0][0] += fp*d2mx*my*mz/(hx*hx);
08779                 dep[1][0] += fp*dmx*dmy*mz/(hy*hx);
08780                 dep[1][1] += fp*mx*d2my*mz/(hy*hy);
08781                 dep[2][0] += fp*dmx*my*dmz/(hx*hzed);
08782                 dep[2][1] += fp*mx*dmy*dmz/(hy*hzed);
08783                 dep[2][2] += fp*mx*my*d2mz/(hzed*hzed);
08784                 /* The 2nd gradient of the field
08785                 VxVxVa */
08786                 d2e[0][0][0] += f*d3mx*my*mz/(hx*hx*hx);
08787                 d2e[0][0][1] += f*d2mx*dmy*mz/(hx*hy*hx);
08788                 d2e[0][0][2] += f*d2mx*my*dmz/(hx*hx*hzed);
08789                 /* VyVxVa */
08790                 d2e[1][0][0] += f*d2mx*dmy*mz/(hx*hx*hy);
08791                 d2e[1][0][1] += f*dmx*d2my*mz/(hx*hy*hy);
08792                 d2e[1][0][2] += f*dmx*dmy*dmz/(hx*hy*hzed);
08793                 /* VyVyVa */
08794                 d2e[1][1][0] += f*dmx*d2my*mz/(hx*hy*hy);
08795                 d2e[1][1][1] += f*mx*d3my*mz/(hy*hy*hy);
08796                 d2e[1][1][2] += f*mx*d2my*dmz/(hy*hy*hzed);
08797                 /* VzVxVa */
08798                 d2e[2][0][0] += f*d2mx*my*dmz/(hx*hx*hzed);
08799                 d2e[2][0][1] += f*dmx*dmy*dmz/(hx*hy*hzed);
08800                 d2e[2][0][2] += f*dmx*my*d2mz/(hx*hzed*hzed);
08801                 /* VzVyVa */
08802                 d2e[2][1][0] += f*dmx*dmy*dmz/(hx*hy*hzed);
08803                 d2e[2][1][1] += f*mx*d2my*dmz/(hy*hy*hzed);
08804                 d2e[2][1][2] += f*mx*dmy*d2mz/(hy*hzed*hzed);
08805                 /* VzVzVa */
08806                 d2e[2][2][0] += f*dmx*my*d2mz/(hx*hzed*hzed);
08807                 d2e[2][2][1] += f*mx*dmy*d2mz/(hy*hzed*hzed);
08808                 d2e[2][2][2] += f*mx*my*d3mz/(hzed*hzed*hzed);
08809             }
08810         }
08811     }
08812 }
08813
08814 /* force on permanent multipole due to induced reaction field */

```

```

08815
08816 /* Monopole Force */
08817 force[0] = e[0]*c;
08818 force[1] = e[1]*c;
08819 force[2] = e[2]*c;
08820
08821 /* Dipole Force */
08822 force[0] -= de[0][0]*ux+de[1][0]*uy+de[2][0]*uz;
08823 force[1] -= de[1][0]*ux+de[1][1]*uy+de[2][1]*uz;
08824 force[2] -= de[2][0]*ux+de[2][1]*uy+de[2][2]*uz;
08825
08826 /* Quadrupole Force */
08827 force[0] += d2e[0][0][0]*qxx
08828           + d2e[1][0][0]*qyx*2.0+d2e[1][1][0]*qyy
08829           + d2e[2][0][0]*qzx*2.0+d2e[2][1][0]*qzy*2.0+d2e[2][2][0]*qzz;
08830 force[1] += d2e[0][0][1]*qxx
08831           + d2e[1][0][1]*qyx*2.0+d2e[1][1][1]*qyy
08832           + d2e[2][0][1]*qzx*2.0+d2e[2][1][1]*qzy*2.0+d2e[2][2][1]*qzz;
08833 force[2] += d2e[0][0][2]*qxx
08834           + d2e[1][0][2]*qyx*2.0+d2e[1][1][2]*qyy
08835           + d2e[2][0][2]*qzx*2.0+d2e[2][1][2]*qzy*2.0+d2e[2][2][2]*qzz;
08836
08837 /* torque on permanent mulitpole due to induced reaction field */
08838
08839 /* Dipole Torque */
08840 torque[0] = uy * e[2] - uz * e[1];
08841 torque[1] = uz * e[0] - ux * e[2];
08842 torque[2] = ux * e[1] - uy * e[0];
08843
08844 /* Quadrupole Torque */
08845 /* Tx = -2.0*(Sum_a (Qya*dEaz) + Sum_b (Qzb*dEby))
08846    Ty = -2.0*(Sum_a (Qza*dEax) + Sum_b (Qxb*dEbz))
08847    Tz = -2.0*(Sum_a (Qxa*dEay) + Sum_b (Qyb*dEbx)) */
08848 de[0][1] = de[1][0];
08849 de[0][2] = de[2][0];
08850 de[1][2] = de[2][1];
08851 torque[0] -= 2.0*(qyx*de[0][2] + qyy*de[1][2] + qyz*de[2][2]
08852                - qzx*de[0][1] - qzy*de[1][1] - qzz*de[2][1]);
08853 torque[1] -= 2.0*(qzx*de[0][0] + qzy*de[1][0] + qzz*de[2][0]
08854                - qxx*de[0][2] - qxy*de[1][2] - qxz*de[2][2]);
08855 torque[2] -= 2.0*(qxx*de[0][1] + qxy*de[1][1] + qxz*de[2][1]
08856                - qyx*de[0][0] - qyy*de[1][0] - qyz*de[2][0]);
08857
08858 /* force on induced dipole due to permanent reaction field */
08859
08860 force[0] -= dep[0][0]*uix+dep[1][0]*uiy+dep[2][0]*uiz;
08861 force[1] -= dep[1][0]*uix+dep[1][1]*uiy+dep[2][1]*uiz;
08862 force[2] -= dep[2][0]*uix+dep[2][1]*uiy+dep[2][2]*uiz;
08863
08864 force[0] = 0.5 * force[0];
08865 force[1] = 0.5 * force[1];
08866 force[2] = 0.5 * force[2];
08867 torque[0] = 0.5 * torque[0];
08868 torque[1] = 0.5 * torque[1];
08869 torque[2] = 0.5 * torque[2];
08870
08871 /* printf(" qPhi Force %f %f %f\n", force[0], force[1], force[2]);
08872    printf(" qPhi Torque %f %f %f\n", torque[0], torque[1], torque[2]); */
08873 }
08874
08875 VPUBLIC void Vpmg_qfNLDirectPolForce(Vpmg *thee, Vgrid *perm, Vgrid *nlInduced,
08876 int atomID, double force[3], double torque[3]) {
08877
08878 Vatom *atom;
08879 double *apos, *dipole, *quad, position[3], hx, hy, hzed;
08880 double xlen, ylen, zlen, xmin, ymin, zmin, xmax, ymax, zmax;
08881 double pot, e[3], de[3][3], dep[3][3], d2e[3][3][3];
08882 double mx, my, mz, dmx, dmy, dmz, mi, mj, mk;
08883 double d2mx, d2my, d2mz, d3mx, d3my, d3mz;
08884 double *u, *up, charge, ifloat, jfloat, kfloat;
08885 double f, fp, c, ux, uy, uz, qxx, qxy, qxz, qyx, qyy, qyz, qzx, qzy, qzz;
08886 double uix, uiy, uiz;
08887 int i,j,k,nx, ny, nz, im2, im1, ip1, ip2, jm2, jm1, jp1, jp2, km2, km1;
08888 int kp1, kp2, ii, jj, kk;
08889
08890 VASSERT(thee != VNULL);
08891 VASSERT(perm != VNULL); /* potential due to permanent multipoles. */
08892 VASSERT(nlInduced != VNULL); /* potential due to non-local induced dipoles */
08893 VASSERT(!thee->pmpg->nonlin); /* Nonlinear PBE is not implemented for AMOEBA */
08894
08895 atom = Valist_getAtom(thee->pbe->alist, atomID);

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08896     VASSERT(atom->partID != 0);    /* Currently all atoms must be in the same partition. */
08897     apos = Vatom_getPosition(atom);
08898
08899     c = Vatom_getCharge(atom);
08900     dipole = Vatom_getDipole(atom);
08901     ux = dipole[0];
08902     uy = dipole[1];
08903     uz = dipole[2];
08904     quad = Vatom_getQuadrupole(atom);
08905     qxx = quad[0]/3.0;
08906     qxy = quad[1]/3.0;
08907     qxz = quad[2]/3.0;
08908     qyx = quad[3]/3.0;
08909     qyy = quad[4]/3.0;
08910     qyz = quad[5]/3.0;
08911     qzx = quad[6]/3.0;
08912     qzy = quad[7]/3.0;
08913     qzz = quad[8]/3.0;
08914
08915     dipole = Vatom_getNLInducedDipole(atom);
08916     uix = dipole[0];
08917     uiy = dipole[1];
08918     uiz = dipole[2];
08919
08920     /* Reset Field Gradients */
08921     pot = 0.0;
08922     for (i=0; i<3; i++){
08923         e[i] = 0.0;
08924         for (j=0; j<3; j++){
08925             de[i][j] = 0.0;
08926             dep[i][j] = 0.0;
08927             for (k=0; k<3; k++){
08928                 d2e[i][j][k] = 0.0;
08929             }
08930         }
08931     }
08932
08933     /* Mesh info */
08934     nx = thee->pmgpp->nx;
08935     ny = thee->pmgpp->ny;
08936     nz = thee->pmgpp->nz;
08937     hx = thee->pmgpp->hx;
08938     hy = thee->pmgpp->hy;
08939     hzed = thee->pmgpp->hzed;
08940     xlen = thee->pmgpp->xlen;
08941     ylen = thee->pmgpp->ylen;
08942     zlen = thee->pmgpp->zlen;
08943     xmin = thee->pmgpp->xmin;
08944     ymin = thee->pmgpp->ymin;
08945     zmin = thee->pmgpp->zmin;
08946     xmax = thee->pmgpp->xmax;
08947     ymax = thee->pmgpp->ymax;
08948     zmax = thee->pmgpp->zmax;
08949     u = nlInduced->data;
08950     up = perm->data;
08951
08952
08953     /* Make sure we're on the grid */
08954     if ((apos[0]<=(xmin+2*hx)) || (apos[0]>=(xmax-2*hx)) \
08955         || (apos[1]<=(ymin+2*hy)) || (apos[1]>=(ymax-2*hy)) \
08956         || (apos[2]<=(zmin+2*hzed)) || (apos[2]>=(zmax-2*hzed))) {
08957         Vnm_print(2, "qfNLDirectMultipoleForce: Atom off the mesh (ignoring) %6.3f %6.3f %6.3f\n",
08958             apos[0], apos[1], apos[2]);
08959     } else {
08960         /* Convert the atom position to grid coordinates */
08961         position[0] = apos[0] - xmin;
08962         position[1] = apos[1] - ymin;
08963         position[2] = apos[2] - zmin;
08964         ifloat = position[0]/hx;
08965         jfloat = position[1]/hy;
08966         kfloat = position[2]/hzed;
08967         ip1 = (int)ceil(ifloat);
08968         ip2 = ip1 + 2;
08969         im1 = (int)floor(ifloat);
08970         im2 = im1 - 2;
08971         jp1 = (int)ceil(jfloat);
08972         jp2 = jp1 + 2;
08973         jm1 = (int)floor(jfloat);
08974         jm2 = jm1 - 2;
08975         kp1 = (int)ceil(kfloat);

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08976     kp2 = kp1 + 2;
08977     km1 = (int)floor(kfloat);
08978     km2 = km1 - 2;
08979
08980     /* This step shouldn't be necessary, but it saves nasty debugging
08981      * later on if something goes wrong */
08982     ip2 = VMIN2(ip2,nx-1);
08983     ip1 = VMIN2(ip1,nx-1);
08984     im1 = VMAX2(im1,0);
08985     im2 = VMAX2(im2,0);
08986     jp2 = VMIN2(jp2,ny-1);
08987     jp1 = VMIN2(jp1,ny-1);
08988     jm1 = VMAX2(jm1,0);
08989     jm2 = VMAX2(jm2,0);
08990     kp2 = VMIN2(kp2,nz-1);
08991     kp1 = VMIN2(kp1,nz-1);
08992     km1 = VMAX2(km1,0);
08993     km2 = VMAX2(km2,0);
08994
08995     for (ii=im2; ii<=ip2; ii++) {
08996         mi = VFCHI4(ii,ifloat);
08997         mx = bspline4(mi);
08998         dmx = dbspline4(mi);
08999         d2mx = d2bspline4(mi);
09000         d3mx = d3bspline4(mi);
09001         for (jj=jm2; jj<=jp2; jj++) {
09002             mj = VFCHI4(jj,jfloat);
09003             my = bspline4(mj);
09004             dmy = dbspline4(mj);
09005             d2my = d2bspline4(mj);
09006             d3my = d3bspline4(mj);
09007             for (kk=km2; kk<=kp2; kk++) {
09008                 mk = VFCHI4(kk,kfloat);
09009                 mz = bspline4(mk);
09010                 dmz = dbspline4(mk);
09011                 d2mz = d2bspline4(mk);
09012                 d3mz = d3bspline4(mk);
09013                 f = u[IJK(ii,jj,kk)];
09014                 fp = up[IJK(ii,jj,kk)];
09015                 /* The potential */
09016                 pot += f*mx*my*mz;
09017                 /* The field */
09018                 e[0] += f*dmx*my*mz/hx;
09019                 e[1] += f*mx*dmy*mz/hy;
09020                 e[2] += f*mx*my*dmz/hzed;
09021                 /* The gradient of the field */
09022                 de[0][0] += f*d2mx*my*mz/(hx*hx);
09023                 de[1][0] += f*dmx*dmy*mz/(hy*hx);
09024                 de[1][1] += f*mx*d2my*mz/(hy*hy);
09025                 de[2][0] += f*dmx*my*dmz/(hx*hzed);
09026                 de[2][1] += f*mx*dmy*dmz/(hy*hzed);
09027                 de[2][2] += f*mx*my*d2mz/(hzed*hzed);
09028                 /* The gradient of the (permanent) field */
09029                 dep[0][0] += fp*d2mx*my*mz/(hx*hx);
09030                 dep[1][0] += fp*dmx*dmy*mz/(hy*hx);
09031                 dep[1][1] += fp*mx*d2my*mz/(hy*hy);
09032                 dep[2][0] += fp*dmx*my*dmz/(hx*hzed);
09033                 dep[2][1] += fp*mx*dmy*dmz/(hy*hzed);
09034                 dep[2][2] += fp*mx*my*d2mz/(hzed*hzed);
09035                 /* The 2nd gradient of the field */
09036                 /* VxVxVa */
09037                 d2e[0][0][0] += f*d3mx*my*mz/(hx*hx*hx);
09038                 d2e[0][0][1] += f*d2mx*dmy*mz/(hx*hy*hx);
09039                 d2e[0][0][2] += f*d2mx*my*dmz/(hx*hx*hzed);
09040                 /* VyVxVa */
09041                 d2e[1][0][0] += f*d2mx*dmy*mz/(hx*hx*hy);
09042                 d2e[1][0][1] += f*dmx*d2my*mz/(hx*hy*hy);
09043                 d2e[1][0][2] += f*dmx*dmy*dmz/(hx*hy*hzed);
09044                 /* VyVyVa */
09045                 d2e[1][1][0] += f*dmx*d2my*mz/(hx*hy*hy);
09046                 d2e[1][1][1] += f*mx*d3my*mz/(hy*hy*hy);
09047                 d2e[1][1][2] += f*mx*d2my*dmz/(hy*hy*hzed);
09048                 /* VzVxVa */
09049                 d2e[2][0][0] += f*d2mx*my*dmz/(hx*hx*hzed);
09050                 d2e[2][0][1] += f*dmx*dmy*dmz/(hx*hy*hzed);
09051                 d2e[2][0][2] += f*dmx*my*d2mz/(hx*hzed*hzed);
09052                 /* VzVyVa */
09053                 d2e[2][1][0] += f*dmx*dmy*dmz/(hx*hy*hzed);
09054                 d2e[2][1][1] += f*mx*d2my*dmz/(hy*hy*hzed);
09055                 d2e[2][1][2] += f*mx*dmy*d2mz/(hy*hzed*hzed);
09056                 /* VzVzVa */

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09057         d2e[2][2][0] += f*dmx*my*d2mz/(hx*hzed*hzed);
09058         d2e[2][2][1] += f*mx*dmy*d2mz/(hy*hzed*hzed);
09059         d2e[2][2][2] += f*mx*my*d3mz/(hzed*hzed*hzed);
09060     }
09061 }
09062 }
09063 }
09064
09065 /* force on permanent multipole due to non-local induced reaction field */
09066
09067 /* Monopole Force */
09068 force[0] = e[0]*c;
09069 force[1] = e[1]*c;
09070 force[2] = e[2]*c;
09071
09072 /* Dipole Force */
09073 force[0] -= de[0][0]*ux+de[1][0]*uy+de[2][0]*uz;
09074 force[1] -= de[1][0]*ux+de[1][1]*uy+de[2][1]*uz;
09075 force[2] -= de[2][0]*ux+de[2][1]*uy+de[2][2]*uz;
09076
09077 /* Quadrupole Force */
09078 force[0] += d2e[0][0][0]*qxx
09079           + d2e[1][0][0]*qyx*2.0+d2e[1][1][0]*qyy
09080           + d2e[2][0][0]*qzx*2.0+d2e[2][1][0]*qzy*2.0+d2e[2][2][0]*qzz;
09081 force[1] += d2e[0][0][1]*qxx
09082           + d2e[1][0][1]*qyx*2.0+d2e[1][1][1]*qyy
09083           + d2e[2][0][1]*qzx*2.0+d2e[2][1][1]*qzy*2.0+d2e[2][2][1]*qzz;
09084 force[2] += d2e[0][0][2]*qxx
09085           + d2e[1][0][2]*qyx*2.0+d2e[1][1][2]*qyy
09086           + d2e[2][0][2]*qzx*2.0+d2e[2][1][2]*qzy*2.0+d2e[2][2][2]*qzz;
09087
09088 /* torque on permanent mulitpole due to non-local induced reaction field */
09089
09090 /* Dipole Torque */
09091 torque[0] = uy * e[2] - uz * e[1];
09092 torque[1] = uz * e[0] - ux * e[2];
09093 torque[2] = ux * e[1] - uy * e[0];
09094
09095 /* Quadrupole Torque */
09096 /* Tx = -2.0*(Sum_a (Qya*dEaz) + Sum_b (Qzb*dEby))
09097    Ty = -2.0*(Sum_a (Qza*dEax) + Sum_b (Qxb*dEbz))
09098    Tz = -2.0*(Sum_a (Qxa*dEay) + Sum_b (Qyb*dEbx)) */
09099 de[0][1] = de[1][0];
09100 de[0][2] = de[2][0];
09101 de[1][2] = de[2][1];
09102 torque[0] -= 2.0*(qyx*de[0][2] + qyy*de[1][2] + qyz*de[2][2]
09103               - qzx*de[0][1] - qzy*de[1][1] - qzz*de[2][1]);
09104 torque[1] -= 2.0*(qzx*de[0][0] + qzy*de[1][0] + qzz*de[2][0]
09105               - qxx*de[0][2] - qxy*de[1][2] - qxz*de[2][2]);
09106 torque[2] -= 2.0*(qxx*de[0][1] + qxy*de[1][1] + qxz*de[2][1]
09107               - qyx*de[0][0] - qyy*de[1][0] - qyz*de[2][0]);
09108
09109 /* force on non-local induced dipole due to permanent reaction field */
09110
09111 force[0] -= dep[0][0]*uix+dep[1][0]*uiy+dep[2][0]*uiz;
09112 force[1] -= dep[1][0]*uix+dep[1][1]*uiy+dep[2][1]*uiz;
09113 force[2] -= dep[2][0]*uix+dep[2][1]*uiy+dep[2][2]*uiz;
09114
09115 force[0] = 0.5 * force[0];
09116 force[1] = 0.5 * force[1];
09117 force[2] = 0.5 * force[2];
09118 torque[0] = 0.5 * torque[0];
09119 torque[1] = 0.5 * torque[1];
09120 torque[2] = 0.5 * torque[2];
09121
09122 /* printf(" qPhi Force %f %f %f\n", force[0], force[1], force[2]);
09123    printf(" qPhi Torque %f %f %f\n", torque[0], torque[1], torque[2]); */
09124 }
09125
09126 VPUBLIC void Vpmg_ibDirectPolForce(Vpmg *thee, Vgrid *perm, Vgrid *induced,
09127 int atomID, double force[3]) {
09128
09129     Vatom *atom;
09130     Valist *alist;
09131     Vacc *acc;
09132     Vpbe *pbe;
09133     Vsurf_Meth srfm;
09134
09135     double *apos, position[3], arad, irad, zkappa2, hx, hy, hzed;
09136     double xlen, ylen, zlen, xmin, ymin, zmin, xmax, ymax, zmax, rtot2;
09137     double rtot, dx, dx2, dy, dy2, dz, dz2, gpos[3], tgrad[3], fmag;

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```

09138     double izmagic;
09139     int i, j, k, nx, ny, nz, imin, imax, jmin, jmax, kmin, kmax;
09140
09141     VASSERT(thee != VNULL);
09142     VASSERT(perm != VNULL); /* potential due to permanent multipoles.*/
09143     VASSERT(induced != VNULL); /* potential due to induced dipoles. */
09144     VASSERT (!thee->pmpg->nonlin); /* Nonlinear PBE is not implemented for AMOEBA */
09145
09146     acc = thee->pbe->acc;
09147     srfrm = thee->surfMeth;
09148     atom = Valist_getAtom(thee->pbe->alist, atomID);
09149     VASSERT(atom->partID != 0); /* Currently all atoms must be in the same partition. */
09150     apos = Vatom_getPosition(atom);
09151     arad = Vatom_getRadius(atom);
09152
09153     /* Reset force */
09154     force[0] = 0.0;
09155     force[1] = 0.0;
09156     force[2] = 0.0;
09157
09158     /* Get PBE info */
09159     pbe = thee->pbe;
09160     acc = pbe->acc;
09161     alist = pbe->alist;
09162     irad = Vpbe_getMaxIonRadius(pbe);
09163     zkappa2 = Vpbe_getZkappa2(pbe);
09164     izmagic = 1.0/Vpbe_getZmagic(pbe);
09165
09166     VASSERT (zkappa2 > VPMGSMALL); /* It is ok to run AMOEBA with no ions, but this is checked for higher
up in the driver. */
09167
09168     /* Mesh info */
09169     nx = induced->nx;
09170     ny = induced->ny;
09171     nz = induced->nz;
09172     hx = induced->hx;
09173     hy = induced->hy;
09174     hzed = induced->hzd;
09175     xmin = induced->xmin;
09176     ymin = induced->ymin;
09177     zmin = induced->zmin;
09178     xmax = induced->xmax;
09179     ymax = induced->ymax;
09180     zmax = induced->zmax;
09181     xlen = xmax-xmin;
09182     ylen = ymax-ymin;
09183     zlen = zmax-zmin;
09184
09185     /* Make sure we're on the grid */
09186     if ((apos[0]<=xmin) || (apos[0]>=xmax) || \
09187         (apos[1]<=ymin) || (apos[1]>=ymax) || \
09188         (apos[2]<=zmin) || (apos[2]>=zmax)) {
09189         Vnm_print(2, "Vpmg_ibForce: Atom at (%4.3f, %4.3f, %4.3f) is off the mesh (ignoring):\n",
09190             apos[0], apos[1], apos[2]);
09191         Vnm_print(2, "Vpmg_ibForce:      xmin = %g, xmax = %g\n", xmin, xmax);
09192         Vnm_print(2, "Vpmg_ibForce:      ymin = %g, ymax = %g\n", ymin, ymax);
09193         Vnm_print(2, "Vpmg_ibForce:      zmin = %g, zmax = %g\n", zmin, zmax);
09194         fflush(stderr);
09195     } else {
09196
09197         /* Convert the atom position to grid reference frame */
09198         position[0] = apos[0] - xmin;
09199         position[1] = apos[1] - ymin;
09200         position[2] = apos[2] - zmin;
09201
09202         /* Integrate over points within this atom's (inflated) radius */
09203         rtot = (irad + arad + thee->splineWin);
09204         rtot2 = VSQR(rtot);
09205         dx = rtot + 0.5*hx;
09206         imin = VMAX2(0, (int)ceil((position[0] - dx)/hx));
09207         imax = VMIN2(nx-1, (int)floor((position[0] + dx)/hx));
09208         for (i=imin; i<=imax; i++) {
09209             dx2 = VSQR(position[0] - hx*i);
09210             if (rtot2 > dx2) dy = VSQRT(rtot2 - dx2) + 0.5*hy;
09211             else dy = 0.5*hy;
09212             jmin = VMAX2(0, (int)ceil((position[1] - dy)/hy));
09213             jmax = VMIN2(ny-1, (int)floor((position[1] + dy)/hy));
09214             for (j=jmin; j<=jmax; j++) {
09215                 dy2 = VSQR(position[1] - hy*j);
09216                 if (rtot2 > (dx2+dy2)) dz = VSQRT(rtot2-dx2-dy2)+0.5*hzed;
09217                 else dz = 0.5*hzed;

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09218         kmin = VMAX2(0, (int)ceil((position[2] - dz)/hzed));
09219         kmax = VMIN2(nz-1, (int)floor((position[2] + dz)/hzed));
09220         for (k=kmin; k<=kmax; k++) {
09221             dz2 = VSQR(k*hzed - position[2]);
09222             /* See if grid point is inside ivdw radius and set ccf
09223              * accordingly (do spline assignment here) */
09224             if ((dz2 + dy2 + dx2) <= rtot2) {
09225                 gpos[0] = i*hx + xmin;
09226                 gpos[1] = j*hy + ymin;
09227                 gpos[2] = k*hzed + zmin;
09228                 Vpmg_splineSelect(srfm, acc, gpos, thee->splineWin, irad,
09229                                 atom, tgrad);
09230                 fmag = induced->data[IJK(i,j,k)];
09231                 fmag *= perm->data[IJK(i,j,k)];
09232                 fmag *= thee->kappa[IJK(i,j,k)];
09233                 force[0] += (zkappa2*fmag*tgrad[0]);
09234                 force[1] += (zkappa2*fmag*tgrad[1]);
09235                 force[2] += (zkappa2*fmag*tgrad[2]);
09236             }
09237         } /* k loop */
09238     } /* j loop */
09239 } /* i loop */
09240 }
09241
09242 force[0] = force[0] * 0.5 * hx * hy * hzed * izmagic;
09243 force[1] = force[1] * 0.5 * hx * hy * hzed * izmagic;
09244 force[2] = force[2] * 0.5 * hx * hy * hzed * izmagic;
09245
09246 }
09247
09248 VPUBLIC void Vpmg_ibNLDirectPolForce(Vpmg *thee, Vgrid *perm, Vgrid *nlInduced,
09249                                     int atomID, double force[3]) {
09250     Vpmg_ibDirectPolForce(thee, perm, nlInduced, atomID, force);
09251 }
09252
09253 VPUBLIC void Vpmg_dbDirectPolForce(Vpmg *thee, Vgrid *perm, Vgrid *induced,
09254                                   int atomID, double force[3]) {
09255
09256     Vatom *atom;
09257     Vacc *acc;
09258     Vpbe *pbe;
09259     Vsurf_Meth srfm;
09260
09261     double *apos, position[3], arad, hx, hy, hzed, izmagic, deps, depsi;
09262     double xlen, ylen, zlen, xmin, ymin, zmin, xmax, ymax, zmax, rtot2, epsp;
09263     double rtot, dx, gpos[3], tgrad[3], dbFmag, epsw, kT;
09264     double *u, *up, Hxijk, Hyijk, Hzijk, Hximljk, Hyijmlk, Hzijkm1;
09265     double dHxijk[3], dHyijk[3], dHzijk[3], dHximljk[3], dHyijmlk[3];
09266     double dHzijkm1[3];
09267     int i, j, k, l, nx, ny, nz, imin, imax, jmin, jmax, kmin, kmax;
09268
09269     VASSERT(thee != VNULL);
09270     VASSERT(perm != VNULL); /* permanent multipole PMG solution. */
09271     VASSERT(induced != VNULL); /* potential due to induced dipoles. */
09272
09273     acc = thee->pbe->acc;
09274     atom = Valist_getAtom(thee->pbe->alist, atomID);
09275     VASSERT (atom->partID != 0); /* Currently all atoms must be in the same partition. */
09276     apos = Vatom_getPosition(atom);
09277     arad = Vatom_getRadius(atom);
09278
09279     /* Reset force */
09280     force[0] = 0.0;
09281     force[1] = 0.0;
09282     force[2] = 0.0;
09283
09284     /* Get PBE info */
09285     pbe = thee->pbe;
09286     acc = pbe->acc;
09287     srfm = thee->surfMeth;
09288     epsp = Vpbe_getSoluteDiel(pbe);
09289     epsw = Vpbe_getSolventDiel(pbe);
09290     kT = Vpbe_getTemperature(pbe)*(1e-3)*Vunit_Na*Vunit_kb;
09291     izmagic = 1.0/Vpbe_getZmagic(pbe);
09292
09293     deps = (epsw - epsp);
09294     depsi = 1.0/deps;
09295     VASSERT (VABS(deps) > VPMGSMALL);
09296
09297     /* Mesh info */
09298     nx = thee->pmgp->nx;

```



```

09299     ny = thee->pmgp->ny;
09300     nz = thee->pmgp->nz;
09301     hx = thee->pmgp->hx;
09302     hy = thee->pmgp->hy;
09303     hzed = thee->pmgp->hzed;
09304     xlen = thee->pmgp->xlen;
09305     ylen = thee->pmgp->ylen;
09306     zlen = thee->pmgp->zlen;
09307     xmin = thee->pmgp->xmin;
09308     ymin = thee->pmgp->ymin;
09309     zmin = thee->pmgp->zmin;
09310     xmax = thee->pmgp->xmax;
09311     ymax = thee->pmgp->ymax;
09312     zmax = thee->pmgp->zmax;
09313     /* If the permanent and induced potentials are flipped the
09314        results are exactly the same. */
09315     u = induced->data;
09316     up = perm->data;
09317
09318     /* Make sure we're on the grid */
09319     if ((apos[0]<=xmin) || (apos[0]>=xmax) || \
09320         (apos[1]<=ymin) || (apos[1]>=ymax) || \
09321         (apos[2]<=zmin) || (apos[2]>=zmax)) {
09322         Vnm_print(2, "Vpmg_dbDirectPolForce: Atom at (%4.3f, %4.3f, %4.3f) is off the mesh
(ignore):\n", apos[0], apos[1], apos[2]);
09323         Vnm_print(2, "Vpmg_dbDirectPolForce:      xmin = %g, xmax = %g\n", xmin, xmax);
09324         Vnm_print(2, "Vpmg_dbDirectPolForce:      ymin = %g, ymax = %g\n", ymin, ymax);
09325         Vnm_print(2, "Vpmg_dbDirectPolForce:      zmin = %g, zmax = %g\n", zmin, zmax);
09326         fflush(stderr);
09327     } else {
09328
09329         /* Convert the atom position to grid reference frame */
09330         position[0] = apos[0] - xmin;
09331         position[1] = apos[1] - ymin;
09332         position[2] = apos[2] - zmin;
09333
09334         /* Integrate over points within this atom's (inflated) radius */
09335         rtot = (arad + thee->splineWin);
09336         rtot2 = VSQR(rtot);
09337         dx = rtot/hx;
09338         imin = (int)floor((position[0]-rtot)/hx);
09339         if (imin < 1) {
09340             Vnm_print(2, "Vpmg_dbDirectPolForce: Atom %d off grid!\n", atomID);
09341             return;
09342         }
09343         imax = (int)ceil((position[0]+rtot)/hx);
09344         if (imax > (nx-2)) {
09345             Vnm_print(2, "Vpmg_dbDirectPolForce: Atom %d off grid!\n", atomID);
09346             return;
09347         }
09348         jmin = (int)floor((position[1]-rtot)/hy);
09349         if (jmin < 1) {
09350             Vnm_print(2, "Vpmg_dbDirectPolForce: Atom %d off grid!\n", atomID);
09351             return;
09352         }
09353         jmax = (int)ceil((position[1]+rtot)/hy);
09354         if (jmax > (ny-2)) {
09355             Vnm_print(2, "Vpmg_dbDirectPolForce: Atom %d off grid!\n", atomID);
09356             return;
09357         }
09358         kmin = (int)floor((position[2]-rtot)/hzed);
09359         if (kmin < 1) {
09360             Vnm_print(2, "Vpmg_dbDirectPolForce: Atom %d off grid!\n", atomID);
09361             return;
09362         }
09363         kmax = (int)ceil((position[2]+rtot)/hzed);
09364         if (kmax > (nz-2)) {
09365             Vnm_print(2, "Vpmg_dbDirectPolForce: Atom %d off grid!\n", atomID);
09366             return;
09367         }
09368         for (i=imin; i<=imax; i++) {
09369             for (j=jmin; j<=jmax; j++) {
09370                 for (k=kmin; k<=kmax; k++) {
09371                     /* i,j,k */
09372                     gpos[0] = (i+0.5)*hx + xmin;
09373                     gpos[1] = j*hy + ymin;
09374                     gpos[2] = k*hzed + zmin;
09375                     Hxijk = (thee->epsx[IJK(i,j,k)] - epsp)*depsi;
09376                     Vpmg_splineSelect(srfm, acc, gpos, thee->splineWin, 0.,
09377                                     atom, dHxijk);
09378                     for (l=0; l<3; l++) dHxijk[l] *= Hxijk;

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09379         gpos[0] = i*hx + xmin;
09380         gpos[1] = (j+0.5)*hy + ymin;
09381         gpos[2] = k*hzed + zmin;
09382         Hyijk = (thee->epsy[IJK(i,j,k)] - epsp)*depsi;
09383         Vpmg_splineSelect(srfm, acc, gpos, thee->splineWin, 0.,
09384             atom, dHyijk);
09385         for (l=0; l<3; l++) dHyijk[l] *= Hyijk;
09386         gpos[0] = i*hx + xmin;
09387         gpos[1] = j*hy + ymin;
09388         gpos[2] = (k+0.5)*hzed + zmin;
09389         Hzijk = (thee->epsz[IJK(i,j,k)] - epsp)*depsi;
09390         Vpmg_splineSelect(srfm, acc, gpos, thee->splineWin, 0.,
09391             atom, dHzijk);
09392         for (l=0; l<3; l++) dHzijk[l] *= Hzijk;
09393         /* i-1,j,k */
09394         gpos[0] = (i-0.5)*hx + xmin;
09395         gpos[1] = j*hy + ymin;
09396         gpos[2] = k*hzed + zmin;
09397         Hximljk = (thee->epsx[IJK(i-1,j,k)] - epsp)*depsi;
09398         Vpmg_splineSelect(srfm, acc, gpos, thee->splineWin, 0.,
09399             atom, dHximljk);
09400         for (l=0; l<3; l++) dHximljk[l] *= Hximljk;
09401         /* i,j-1,k */
09402         gpos[0] = i*hx + xmin;
09403         gpos[1] = (j-0.5)*hy + ymin;
09404         gpos[2] = k*hzed + zmin;
09405         Hyijmlk = (thee->epsy[IJK(i,j-1,k)] - epsp)*depsi;
09406         Vpmg_splineSelect(srfm, acc, gpos, thee->splineWin, 0.,
09407             atom, dHyijmlk);
09408         for (l=0; l<3; l++) dHyijmlk[l] *= Hyijmlk;
09409         /* i,j,k-1 */
09410         gpos[0] = i*hx + xmin;
09411         gpos[1] = j*hy + ymin;
09412         gpos[2] = (k-0.5)*hzed + zmin;
09413         Hzijkm1 = (thee->epsz[IJK(i,j,k-1)] - epsp)*depsi;
09414         Vpmg_splineSelect(srfm, acc, gpos, thee->splineWin, 0.,
09415             atom, dHzijkm1);
09416         for (l=0; l<3; l++) dHzijkm1[l] *= Hzijkm1;
09417
09418         dbFmag = up[IJK(i,j,k)];
09419         tgrad[0] =
09420             (dHxijk[0] * (u[IJK(i+1,j,k)]-u[IJK(i,j,k)]))
09421             + dHximljk[0] * (u[IJK(i-1,j,k)]-u[IJK(i,j,k)])) /VSQR(hx)
09422             + (dHyijk[0] * (u[IJK(i,j+1,k)]-u[IJK(i,j,k)]))
09423             + dHyijmlk[0] * (u[IJK(i,j-1,k)]-u[IJK(i,j,k)])) /VSQR(hy)
09424             + (dHzijk[0] * (u[IJK(i,j,k+1)]-u[IJK(i,j,k)]))
09425             + dHzijkm1[0] * (u[IJK(i,j,k-1)]-u[IJK(i,j,k)])) /VSQR(hzed);
09426         tgrad[1] =
09427             (dHxijk[1] * (u[IJK(i+1,j,k)]-u[IJK(i,j,k)]))
09428             + dHximljk[1] * (u[IJK(i-1,j,k)]-u[IJK(i,j,k)])) /VSQR(hx)
09429             + (dHyijk[1] * (u[IJK(i,j+1,k)]-u[IJK(i,j,k)]))
09430             + dHyijmlk[1] * (u[IJK(i,j-1,k)]-u[IJK(i,j,k)])) /VSQR(hy)
09431             + (dHzijk[1] * (u[IJK(i,j,k+1)]-u[IJK(i,j,k)]))
09432             + dHzijkm1[1] * (u[IJK(i,j,k-1)]-u[IJK(i,j,k)])) /VSQR(hzed);
09433         tgrad[2] =
09434             (dHxijk[2] * (u[IJK(i+1,j,k)]-u[IJK(i,j,k)]))
09435             + dHximljk[2] * (u[IJK(i-1,j,k)]-u[IJK(i,j,k)])) /VSQR(hx)
09436             + (dHyijk[2] * (u[IJK(i,j+1,k)]-u[IJK(i,j,k)]))
09437             + dHyijmlk[2] * (u[IJK(i,j-1,k)]-u[IJK(i,j,k)])) /VSQR(hy)
09438             + (dHzijk[2] * (u[IJK(i,j,k+1)]-u[IJK(i,j,k)]))
09439             + dHzijkm1[2] * (u[IJK(i,j,k-1)]-u[IJK(i,j,k)])) /VSQR(hzed);
09440         force[0] += (dbFmag*tgrad[0]);
09441         force[1] += (dbFmag*tgrad[1]);
09442         force[2] += (dbFmag*tgrad[2]);
09443
09444         } /* k loop */
09445     } /* j loop */
09446 } /* i loop */
09447
09448     force[0] = -force[0]*hx*hy*hzed*deps*0.5*izmagic;
09449     force[1] = -force[1]*hx*hy*hzed*deps*0.5*izmagic;
09450     force[2] = -force[2]*hx*hy*hzed*deps*0.5*izmagic;
09451
09452 }
09453 }
09454
09455 VPUBLIC void Vpmg_dbNLDirectPolForce(Vpmg *thee, Vgrid *perm, Vgrid *nlInduced,
09456     int atomID, double force[3]) {
09457     Vpmg_dbDirectPolForce(thee, perm, nlInduced, atomID, force);
09458 }
09459

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09460 VPUBLIC void Vpmg_qfMutualPolForce(Vpmg *thee, Vgrid *induced,
09461                                     Vgrid *nlanduced, int atomID, double force[3]) {
09462
09463     Vatom *atom;
09464     double *apos, *dipole, position[3], hx, hy, hzed;
09465     double *u, *unl;
09466     double xlen, ylen, zlen, xmin, ymin, zmin, xmax, ymax, zmax;
09467     double de[3][3], denl[3][3];
09468     double mx, my, mz, dmX, dmy, dmz, d2mx, d2my, d2mz, mi, mj, mk;
09469     double ifloat, jfloat, kfloat;
09470     double f, fnl, uix, uiy, uiz, uixnl, uiynl, uiznl;
09471     int i,j,k,nx, ny, nz, im2, im1, ip1, ip2, jm2, jm1, jp1, jp2, km2, km1;
09472     int kp1, kp2, ii, jj, kk;
09473
09474     VASSERT(thee != VNULL); /* PMG object with PBE info. */
09475     VASSERT(induced != VNULL); /* potential due to induced dipoles. */
09476     VASSERT(nlanduced != VNULL); /* potential due to non-local induced dipoles. */
09477     atom = Valist_getAtom(thee->pbe->alist, atomID);
09478     VASSERT(atom->partID != 0); /* all atoms must be in the same partition. */
09479     apos = Vatom_getPosition(atom);
09480     dipole = Vatom_getInducedDipole(atom);
09481     uix = dipole[0];
09482     uiy = dipole[1];
09483     uiz = dipole[2];
09484     dipole = Vatom_getNLInducedDipole(atom);
09485     uixnl = dipole[0];
09486     uiynl = dipole[1];
09487     uiznl = dipole[2];
09488     u = induced->data;
09489     unl = nlanduced->data;
09490
09491     for (i=0;i<3;i++){
09492         for (j=0;j<3;j++){
09493             de[i][j] = 0.0;
09494             denl[i][j] = 0.0;
09495         }
09496     }
09497
09498     /* Mesh info */
09499     nx = induced->nx;
09500     ny = induced->ny;
09501     nz = induced->nz;
09502     hx = induced->hx;
09503     hy = induced->hy;
09504     hzed = induced->hzed;
09505     xmin = induced->xmin;
09506     ymin = induced->ymin;
09507     zmin = induced->zmin;
09508     xmax = induced->xmax;
09509     ymax = induced->ymax;
09510     zmax = induced->zmax;
09511     xlen = xmax-xmin;
09512     ylen = ymax-ymin;
09513     zlen = zmax-zmin;
09514
09515     /* If we aren't in the current position, then we're done */
09516     if (atom->partID == 0) return;
09517
09518     /* Make sure we're on the grid */
09519     if ((apos[0]<=(xmin+2*hx)) || (apos[0]>=(xmax-2*hx)) \
09520         || (apos[1]<=(ymin+2*hy)) || (apos[1]>=(ymax-2*hy)) \
09521         || (apos[2]<=(zmin+2*hzed)) || (apos[2]>=(zmax-2*hzed))) {
09522         Vnm_print(2, "qfMutualPolForce: Atom off the mesh (ignoring) %6.3f %6.3f %6.3f\n", apos[0],
09523         apos[1], apos[2]);
09524         fflush(stderr);
09525     } else {
09526         /* Convert the atom position to grid coordinates */
09527         position[0] = apos[0] - xmin;
09528         position[1] = apos[1] - ymin;
09529         position[2] = apos[2] - zmin;
09530         ifloat = position[0]/hx;
09531         jfloat = position[1]/hy;
09532         kfloat = position[2]/hzed;
09533         ip1 = (int)ceil(ifloat);
09534         ip2 = ip1 + 2;
09535         im1 = (int)floor(ifloat);
09536         im2 = im1 - 2;
09537         jp1 = (int)ceil(jfloat);
09538         jp2 = jp1 + 2;
09539         jm1 = (int)floor(jfloat);

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09540         jm2 = jm1 - 2;
09541         kp1 = (int)ceil(kfloat);
09542         kp2 = kp1 + 2;
09543         km1 = (int)floor(kfloat);
09544         km2 = km1 - 2;
09545
09546         /* This step shouldn't be necessary, but it saves nasty debugging
09547          * later on if something goes wrong */
09548         ip2 = VMIN2(ip2,nx-1);
09549         ip1 = VMIN2(ip1,nx-1);
09550         im1 = VMAX2(im1,0);
09551         im2 = VMAX2(im2,0);
09552         jp2 = VMIN2(jp2,ny-1);
09553         jp1 = VMIN2(jp1,ny-1);
09554         jm1 = VMAX2(jm1,0);
09555         jm2 = VMAX2(jm2,0);
09556         kp2 = VMIN2(kp2,nz-1);
09557         kp1 = VMIN2(kp1,nz-1);
09558         km1 = VMAX2(km1,0);
09559         km2 = VMAX2(km2,0);
09560
09561         for (ii=im2; ii<=ip2; ii++) {
09562             mi = VFCHI4(ii,ifloat);
09563             mx = bspline4(mi);
09564             dmx = dbspline4(mi);
09565             d2mx = d2bspline4(mi);
09566             for (jj=jm2; jj<=jp2; jj++) {
09567                 mj = VFCHI4(jj,jfloat);
09568                 my = bspline4(mj);
09569                 dmy = dbspline4(mj);
09570                 d2my = d2bspline4(mj);
09571                 for (kk=km2; kk<=kp2; kk++) {
09572                     mk = VFCHI4(kk,kfloat);
09573                     mz = bspline4(mk);
09574                     dmz = dbspline4(mk);
09575                     d2mz = d2bspline4(mk);
09576                     f = u[IJK(ii,jj,kk)];
09577                     fnl = unl[IJK(ii,jj,kk)];
09578
09579                     /* The gradient of the reaction field
09580                      due to induced dipoles */
09581                     de[0][0] += f*d2mx*my*mz/(hx*hx);
09582                     de[1][0] += f*dmx*dmy*mz/(hy*hx);
09583                     de[1][1] += f*mx*d2my*mz/(hy*hy);
09584                     de[2][0] += f*dmx*my*dmz/(hx*hzed);
09585                     de[2][1] += f*mx*dmy*dmz/(hy*hzed);
09586                     de[2][2] += f*mx*my*d2mz/(hzed*hzed);
09587
09588                     /* The gradient of the reaction field
09589                      due to non-local induced dipoles */
09590                     denl[0][0] += fnl*d2mx*my*mz/(hx*hx);
09591                     denl[1][0] += fnl*dmx*dmy*mz/(hy*hx);
09592                     denl[1][1] += fnl*mx*d2my*mz/(hy*hy);
09593                     denl[2][0] += fnl*dmx*my*dmz/(hx*hzed);
09594                     denl[2][1] += fnl*mx*dmy*dmz/(hy*hzed);
09595                     denl[2][2] += fnl*mx*my*d2mz/(hzed*hzed);
09596                 }
09597             }
09598         }
09599     }
09600
09601     /* mutual polarization force */
09602     force[0] = -(de[0][0]*uixnl + de[1][0]*uiynl + de[2][0]*uiznl);
09603     force[1] = -(de[1][0]*uixnl + de[1][1]*uiynl + de[2][1]*uiznl);
09604     force[2] = -(de[2][0]*uixnl + de[2][1]*uiynl + de[2][2]*uiznl);
09605     force[0] -= denl[0][0]*uix + denl[1][0]*uiy + denl[2][0]*uiz;
09606     force[1] -= denl[1][0]*uix + denl[1][1]*uiy + denl[2][1]*uiz;
09607     force[2] -= denl[2][0]*uix + denl[2][1]*uiy + denl[2][2]*uiz;
09608
09609     force[0] = 0.5 * force[0];
09610     force[1] = 0.5 * force[1];
09611     force[2] = 0.5 * force[2];
09612 }
09613
09614
09615 VPUBLIC void Vpmg_ibMutualPolForce(Vpmg *thee, Vgrid *induced, Vgrid *nlinduced,
09616                                   int atomID, double force[3]) {
09617
09618     Vatom *atom;
09619     Valist *alist;
09620     Vacc *acc;

```

```

09621     Vpbe *pbe;
09622     Vsurf_Meth srfm;
09623
09624     double *apos, position[3], arad, irad, zkappa2, hx, hy, hzed;
09625     double xlen, ylen, zlen, xmin, ymin, zmin, xmax, ymax, zmax, rtot2;
09626     double rtot, dx, dx2, dy, dy2, dz, dz2, gpos[3], tgrad[3], fmag;
09627     double izmagic;
09628     int i, j, k, nx, ny, nz, imin, imax, jmin, jmax, kmin, kmax;
09629
09630     VASSERT(thee != VNULL);          /* We need a PMG object with PBE info. */
09631     VASSERT(induced != VNULL);       /* We need the potential due to induced dipoles. */
09632     VASSERT(nlinduced != VNULL);     /* We need the potential due to non-local induced dipoles. */
09633     VASSERT(!thee->pmpg->nonlin);    /* Nonlinear PBE is not implemented for AMOEBA */
09634
09635     atom = Valist_getAtom(thee->pbe->alist, atomID);
09636     VASSERT (atom->partID != 0);      /* Currently all atoms must be in the same partition. */
09637
09638     acc = thee->pbe->acc;
09639     srfm = thee->surfMeth;
09640     apos = Vatom_getPosition(atom);
09641     arad = Vatom_getRadius(atom);
09642
09643     /* Reset force */
09644     force[0] = 0.0;
09645     force[1] = 0.0;
09646     force[2] = 0.0;
09647
09648     /* If we aren't in the current position, then we're done */
09649     if (atom->partID == 0) return;
09650
09651     /* Get PBE info */
09652     pbe = thee->pbe;
09653     acc = pbe->acc;
09654     alist = pbe->alist;
09655     irad = Vpbe_getMaxIonRadius(pbe);
09656     zkappa2 = Vpbe_getZkappa2(pbe);
09657     izmagic = 1.0/Vpbe_getZmagic(pbe);
09658
09659     VASSERT (zkappa2 > VPMGSMALL); /* Should be a check for this further up.*/
09660
09661     /* Mesh info */
09662     nx = induced->nx;
09663     ny = induced->ny;
09664     nz = induced->nz;
09665     hx = induced->hx;
09666     hy = induced->hy;
09667     hzed = induced->hzed;
09668     xmin = induced->xmin;
09669     ymin = induced->ymin;
09670     zmin = induced->zmin;
09671     xmax = induced->xmax;
09672     ymax = induced->ymax;
09673     zmax = induced->zmax;
09674     xlen = xmax-xmin;
09675     ylen = ymax-ymin;
09676     zlen = zmax-zmin;
09677
09678     /* Make sure we're on the grid */
09679     if ((apos[0]<=xmin) || (apos[0]>=xmax) || \
09680         (apos[1]<=ymin) || (apos[1]>=ymax) || \
09681         (apos[2]<=zmin) || (apos[2]>=zmax)) {
09682         Vnm_print(2, "Vpmg_ibMutalPolForce: Atom at (%4.3f, %4.3f, %4.3f) is off the mesh (ignoring):\n",
09683             apos[0], apos[1], apos[2]);
09684         Vnm_print(2, "Vpmg_ibMutalPolForce: xmin = %g, xmax = %g\n", xmin, xmax);
09685         Vnm_print(2, "Vpmg_ibMutalPolForce: ymin = %g, ymax = %g\n", ymin, ymax);
09686         Vnm_print(2, "Vpmg_ibMutalPolForce: zmin = %g, zmax = %g\n", zmin, zmax);
09687         fflush(stderr);
09688     } else {
09689         /* Convert the atom position to grid reference frame */
09690         position[0] = apos[0] - xmin;
09691         position[1] = apos[1] - ymin;
09692         position[2] = apos[2] - zmin;
09693
09694         /* Integrate over points within this atom's (inflated) radius */
09695         rtot = (irad + arad + thee->splineWin);
09696         rtot2 = VSQR(rtot);
09697         dx = rtot + 0.5*hx;
09698         imin = VMAX2(0, (int)ceil((position[0] - dx)/hx));
09699         imax = VMIN2(nx-1, (int)floor((position[0] + dx)/hx));
09700         for (i=imin; i<=imax; i++) {

```

```

09701         dx2 = VSQR(position[0] - hx*i);
09702         if (rtot2 > dx2) dy = VSQRT(rtot2 - dx2) + 0.5*hy;
09703         else dy = 0.5*hy;
09704         jmin = VMAX2(0, (int)ceil((position[1] - dy)/hy));
09705         jmax = VMIN2(ny-1, (int)floor((position[1] + dy)/hy));
09706         for (j=jmin; j<=jmax; j++) {
09707             dy2 = VSQR(position[1] - hy*j);
09708             if (rtot2 > (dx2+dy2)) dz = VSQRT(rtot2-dx2-dy2)+0.5*hzed;
09709             else dz = 0.5*hzed;
09710             kmin = VMAX2(0, (int)ceil((position[2] - dz)/hzed));
09711             kmax = VMIN2(nz-1, (int)floor((position[2] + dz)/hzed));
09712             for (k=kmin; k<=kmax; k++) {
09713                 dz2 = VSQR(k*hzed - position[2]);
09714                 /* See if grid point is inside ivdw radius and set ccf
09715                  * accordingly (do spline assignment here) */
09716                 if ((dz2 + dy2 + dx2) <= rtot2) {
09717                     gpos[0] = i*hx + xmin;
09718                     gpos[1] = j*hy + ymin;
09719                     gpos[2] = k*hzed + zmin;
09720                     Vpmg_splineSelect(srfm, acc, gpos, thee->splineWin, irad,
09721                                     atom, tgrad);
09722                     fmag = induced->data[IJK(i,j,k)];
09723                     fmag *= nlinduced->data[IJK(i,j,k)];
09724                     fmag *= thee->kappa[IJK(i,j,k)];
09725                     force[0] += (zkappa2*fmag*tgrad[0]);
09726                     force[1] += (zkappa2*fmag*tgrad[1]);
09727                     force[2] += (zkappa2*fmag*tgrad[2]);
09728                 }
09729             } /* k loop */
09730         } /* j loop */
09731     } /* i loop */
09732 }
09733
09734 force[0] = force[0] * 0.5 * hx * hy * hzed * izmagic;
09735 force[1] = force[1] * 0.5 * hx * hy * hzed * izmagic;
09736 force[2] = force[2] * 0.5 * hx * hy * hzed * izmagic;
09737 }
09738
09739 VPUBLIC void Vpmg_dbMutualPolForce(Vpmg *thee, Vgrid *induced,
09740                                   Vgrid *nlinduced, int atomID,
09741                                   double force[3]) {
09742
09743     Vatom *atom;
09744     Vacc *acc;
09745     Vpbe *pbe;
09746     Vsurf_Meth srfm;
09747
09748     double *apos, position[3], arad, hx, hy, hzed, izmagic, deps, deps;
09749     double xlen, ylen, zlen, xmin, ymin, zmin, xmax, ymax, zmax, rtot2, epsp;
09750     double rtot, dx, gpos[3], tgrad[3], dbFmag, epsw, kT;
09751     double *u, *unl, Hxijk, Hyijk, Hzijk, Hximljk, Hyijmlk, Hzijkm1;
09752     double dHxijk[3], dHyijk[3], dHzijk[3], dHximljk[3], dHyijmlk[3];
09753     double dHzijkm1[3];
09754     int i, j, k, l, nx, ny, nz, imin, imax, jmin, jmax, kmin, kmax;
09755
09756     VASSERT(thee != VNULL); /* PMG object with PBE info. */
09757     VASSERT(induced != VNULL); /* potential due to induced dipoles.*/
09758     VASSERT(nlinduced != VNULL); /* potential due to non-local induced dipoles.*/
09759
09760     acc = thee->pbe->acc;
09761     srfm = thee->surfMeth;
09762     atom = Valist_getAtom(thee->pbe->alist, atomID);
09763     VASSERT (atom->partID != 0); /* all atoms must be in the same partition.*/
09764     apos = Vatom_getPosition(atom);
09765     arad = Vatom_getRadius(atom);
09766
09767     /* Reset force */
09768     force[0] = 0.0;
09769     force[1] = 0.0;
09770     force[2] = 0.0;
09771
09772     /* Get PBE info */
09773     pbe = thee->pbe;
09774     acc = pbe->acc;
09775     epsp = Vpbe_getSoluteDiel(pbe);
09776     epsw = Vpbe_getSolventDiel(pbe);
09777     kT = Vpbe_getTemperature(pbe)*(1e-3)*Vunit_Na*Vunit_kb;
09778     izmagic = 1.0/Vpbe_getZmagic(pbe);
09779
09780     deps = (epsw - epsp);
09781     deps = 1.0/deps;

```

```

09782     VASSERT(VABS(deps) > VPMGSMALL);
09783
09784     /* Mesh info */
09785     nx = thee->pmgp->nx;
09786     ny = thee->pmgp->ny;
09787     nz = thee->pmgp->nz;
09788     hx = thee->pmgp->hx;
09789     hy = thee->pmgp->hy;
09790     hzed = thee->pmgp->hzed;
09791     xlen = thee->pmgp->xlen;
09792     ylen = thee->pmgp->ylen;
09793     zlen = thee->pmgp->zlen;
09794     xmin = thee->pmgp->xmin;
09795     ymin = thee->pmgp->ymin;
09796     zmin = thee->pmgp->zmin;
09797     xmax = thee->pmgp->xmax;
09798     ymax = thee->pmgp->ymax;
09799     zmax = thee->pmgp->zmax;
09800     u = induced->data;
09801     unl = nlinduced->data;
09802
09803     /* Make sure we're on the grid */
09804     if ((apos[0]<=xmin) || (apos[0]>=xmax) || \
09805         (apos[1]<=ymin) || (apos[1]>=ymax) || \
09806         (apos[2]<=zmin) || (apos[2]>=zmax)) {
09807         Vnm_print(2, "Vpmg_dbMutualPolForce: Atom at (%4.3f, %4.3f, %4.3f) is off the mesh
09808 (ignoring):\n", apos[0], apos[1], apos[2]);
09809         Vnm_print(2, "Vpmg_dbMutualPolForce:      xmin = %g, xmax = %g\n", xmin, xmax);
09810         Vnm_print(2, "Vpmg_dbMutualPolForce:      ymin = %g, ymax = %g\n", ymin, ymax);
09811         Vnm_print(2, "Vpmg_dbMutualPolForce:      zmin = %g, zmax = %g\n", zmin, zmax);
09812     } else {
09813
09814         /* Convert the atom position to grid reference frame */
09815         position[0] = apos[0] - xmin;
09816         position[1] = apos[1] - ymin;
09817         position[2] = apos[2] - zmin;
09818
09819         /* Integrate over points within this atom's (inflated) radius */
09820         rtot = (arad + thee->splineWin);
09821         rtot2 = VSQR(rtot);
09822         dx = rtot/hx;
09823         imin = (int)floor((position[0]-rtot)/hx);
09824         if (imin < 1) {
09825             Vnm_print(2, "Vpmg_dbMutualPolForce: Atom %d off grid!\n", atomID);
09826             return;
09827         }
09828         imax = (int)ceil((position[0]+rtot)/hx);
09829         if (imax > (nx-2)) {
09830             Vnm_print(2, "Vpmg_dbMutualPolForce: Atom %d off grid!\n", atomID);
09831             return;
09832         }
09833         jmin = (int)floor((position[1]-rtot)/hy);
09834         if (jmin < 1) {
09835             Vnm_print(2, "Vpmg_dbMutualPolForce: Atom %d off grid!\n", atomID);
09836             return;
09837         }
09838         jmax = (int)ceil((position[1]+rtot)/hy);
09839         if (jmax > (ny-2)) {
09840             Vnm_print(2, "Vpmg_dbMutualPolForce: Atom %d off grid!\n", atomID);
09841             return;
09842         }
09843         kmin = (int)floor((position[2]-rtot)/hzed);
09844         if (kmin < 1) {
09845             Vnm_print(2, "Vpmg_dbMutualPolForce: Atom %d off grid!\n", atomID);
09846             return;
09847         }
09848         kmax = (int)ceil((position[2]+rtot)/hzed);
09849         if (kmax > (nz-2)) {
09850             Vnm_print(2, "Vpmg_dbMutualPolForce: Atom %d off grid!\n", atomID);
09851             return;
09852         }
09853         for (i=imin; i<=imax; i++) {
09854             for (j=jmin; j<=jmax; j++) {
09855                 for (k=kmin; k<=kmax; k++) {
09856                     /* i,j,k */
09857                     gpos[0] = (i+0.5)*hx + xmin;
09858                     gpos[1] = j*hy + ymin;
09859                     gpos[2] = k*hzed + zmin;
09860                     Hxijk = (thee->epsx[IJK(i,j,k)] - epsp)*depsi;
09861                     Vpmg_splineSelect(srfm, acc, gpos, thee->splineWin, 0.,

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```

09862         atom, dHxijk);
09863     for (l=0; l<3; l++) dHxijk[l] *= Hxijk;
09864     gpos[0] = i*hx + xmin;
09865     gpos[1] = (j+0.5)*hy + ymin;
09866     gpos[2] = k*hzed + zmin;
09867     Hyijk = (thee->epsy[IJK(i,j,k)] - epsp)*depsi;
09868     Vpmg_splineSelect(srfm, acc, gpos, thee->splineWin, 0.,
09869         atom, dHyijk);
09870     for (l=0; l<3; l++) dHyijk[l] *= Hyijk;
09871     gpos[0] = i*hx + xmin;
09872     gpos[1] = j*hy + ymin;
09873     gpos[2] = (k+0.5)*hzed + zmin;
09874     Hzijk = (thee->epsz[IJK(i,j,k)] - epsp)*depsi;
09875     Vpmg_splineSelect(srfm, acc, gpos, thee->splineWin, 0.,
09876         atom, dHzijk);
09877     for (l=0; l<3; l++) dHzijk[l] *= Hzijk;
09878     /* i-1,j,k */
09879     gpos[0] = (i-0.5)*hx + xmin;
09880     gpos[1] = j*hy + ymin;
09881     gpos[2] = k*hzed + zmin;
09882     Hximljk = (thee->epsx[IJK(i-1,j,k)] - epsp)*depsi;
09883     Vpmg_splineSelect(srfm, acc, gpos, thee->splineWin, 0.,
09884         atom, dHximljk);
09885     for (l=0; l<3; l++) dHximljk[l] *= Hximljk;
09886     /* i,j-1,k */
09887     gpos[0] = i*hx + xmin;
09888     gpos[1] = (j-0.5)*hy + ymin;
09889     gpos[2] = k*hzed + zmin;
09890     Hyijmlk = (thee->epsy[IJK(i,j-1,k)] - epsp)*depsi;
09891     Vpmg_splineSelect(srfm, acc, gpos, thee->splineWin, 0.,
09892         atom, dHyijmlk);
09893     for (l=0; l<3; l++) dHyijmlk[l] *= Hyijmlk;
09894     /* i,j,k-1 */
09895     gpos[0] = i*hx + xmin;
09896     gpos[1] = j*hy + ymin;
09897     gpos[2] = (k-0.5)*hzed + zmin;
09898     Hzijkml = (thee->epsz[IJK(i,j,k-1)] - epsp)*depsi;
09899     Vpmg_splineSelect(srfm, acc, gpos, thee->splineWin, 0.,
09900         atom, dHzijkml);
09901     for (l=0; l<3; l++) dHzijkml[l] *= Hzijkml;
09902     dbFmag = unl[IJK(i,j,k)];
09903     tgrad[0] =
09904         (dHxijk[0] * (u[IJK(i+1,j,k)]-u[IJK(i,j,k)])
09905         + dHximljk[0] * (u[IJK(i-1,j,k)]-u[IJK(i,j,k)])) /VSQR(hx)
09906         + (dHyijk[0] * (u[IJK(i,j+1,k)]-u[IJK(i,j,k)])
09907         + dHyijmlk[0] * (u[IJK(i,j-1,k)]-u[IJK(i,j,k)])) /VSQR(hy)
09908         + (dHzijk[0] * (u[IJK(i,j,k+1)]-u[IJK(i,j,k)])
09909         + dHzijkml[0] * (u[IJK(i,j,k-1)]-u[IJK(i,j,k)])) /VSQR(hzed);
09910     tgrad[1] =
09911         (dHxijk[1] * (u[IJK(i+1,j,k)]-u[IJK(i,j,k)])
09912         + dHximljk[1] * (u[IJK(i-1,j,k)]-u[IJK(i,j,k)])) /VSQR(hx)
09913         + (dHyijk[1] * (u[IJK(i,j+1,k)]-u[IJK(i,j,k)])
09914         + dHyijmlk[1] * (u[IJK(i,j-1,k)]-u[IJK(i,j,k)])) /VSQR(hy)
09915         + (dHzijk[1] * (u[IJK(i,j,k+1)]-u[IJK(i,j,k)])
09916         + dHzijkml[1] * (u[IJK(i,j,k-1)]-u[IJK(i,j,k)])) /VSQR(hzed);
09917     tgrad[2] =
09918         (dHxijk[2] * (u[IJK(i+1,j,k)]-u[IJK(i,j,k)])
09919         + dHximljk[2] * (u[IJK(i-1,j,k)]-u[IJK(i,j,k)])) /VSQR(hx)
09920         + (dHyijk[2] * (u[IJK(i,j+1,k)]-u[IJK(i,j,k)])
09921         + dHyijmlk[2] * (u[IJK(i,j-1,k)]-u[IJK(i,j,k)])) /VSQR(hy)
09922         + (dHzijk[2] * (u[IJK(i,j,k+1)]-u[IJK(i,j,k)])
09923         + dHzijkml[2] * (u[IJK(i,j,k-1)]-u[IJK(i,j,k)])) /VSQR(hzed);
09924     force[0] += (dbFmag*tgrad[0]);
09925     force[1] += (dbFmag*tgrad[1]);
09926     force[2] += (dbFmag*tgrad[2]);
09927     } /* k loop */
09928     } /* j loop */
09929     } /* i loop */
09930
09931     force[0] = -force[0]*hx*hy*hzed*deps*0.5*izmagic;
09932     force[1] = -force[1]*hx*hy*hzed*deps*0.5*izmagic;
09933     force[2] = -force[2]*hx*hy*hzed*deps*0.5*izmagic;
09934 }
09935 }
09936
09937 #endif /* if defined(WITH_TINKER) */
09938
09939 VPRIVATE void fillCoefSpline4(Vpmg *thee) {
09940
09941     Valist *alist;
09942     Vpbe *pbe;

```



```

09943     Vatom *atom;
09944     double xmin, xmax, ymin, ymax, zmin, zmax, ionmask, ionstr, dist2;
09945     double xlen, ylen, zlen, position[3], itot, stot, ictot, ictot2, sctot;
09946     double irad, dx, dy, dz, epsw, epsp, w2i;
09947     double hx, hy, hzed, *apos, arad, sctot2;
09948     double dx2, dy2, dz2, stot2, itot2, rtot, rtot2, splineWin;
09949     double dist, value, denom, sm, sm2, sm3, sm4, sm5, sm6, sm7;
09950     double e, e2, e3, e4, e5, e6, e7;
09951     double b, b2, b3, b4, b5, b6, b7;
09952     double c0, c1, c2, c3, c4, c5, c6, c7;
09953     double ic0, ic1, ic2, ic3, ic4, ic5, ic6, ic7;
09954     int i, j, k, nx, ny, nz, iatom;
09955     int imin, imax, jmin, jmax, kmin, kmax;
09956
09957     VASSERT(thee != VNULL);
09958     splineWin = thee->splineWin;
09959
09960     /* Get PBE info */
09961     pbe = thee->pbe;
09962     alist = pbe->alist;
09963     irad = Vpbe_getMaxIonRadius(pbe);
09964     ionstr = Vpbe_getBulkIonicStrength(pbe);
09965     epsw = Vpbe_getSolventDiel(pbe);
09966     epsp = Vpbe_getSoluteDiel(pbe);
09967
09968     /* Mesh info */
09969     nx = thee->pmgp->nx;
09970     ny = thee->pmgp->ny;
09971     nz = thee->pmgp->nz;
09972     hx = thee->pmgp->hx;
09973     hy = thee->pmgp->hy;
09974     hzed = thee->pmgp->hzed;
09975
09976     /* Define the total domain size */
09977     xlen = thee->pmgp->xlen;
09978     ylen = thee->pmgp->ylen;
09979     zlen = thee->pmgp->zlen;
09980
09981     /* Define the min/max dimensions */
09982     xmin = thee->pmgp->xcent - (xlen/2.0);
09983     ymin = thee->pmgp->ycent - (ylen/2.0);
09984     zmin = thee->pmgp->zcent - (zlen/2.0);
09985     xmax = thee->pmgp->xcent + (xlen/2.0);
09986     ymax = thee->pmgp->ycent + (ylen/2.0);
09987     zmax = thee->pmgp->zcent + (zlen/2.0);
09988
09989     /* This is a floating point parameter related to the non-zero nature of the
09990      * bulk ionic strength. If the ionic strength is greater than zero; this
09991      * parameter is set to 1.0 and later scaled by the appropriate pre-factors.
09992      * Otherwise, this parameter is set to 0.0 */
09993     if (ionstr > VPMGSMALL) ionmask = 1.0;
09994     else ionmask = 0.0;
09995
09996     /* Reset the kappa, epsx, epsy, and epsz arrays */
09997     for (i=0; i<(nx*ny*nz); i++) {
09998         thee->kappa[i] = 1.0;
09999         thee->epsx[i] = 1.0;
10000         thee->epsy[i] = 1.0;
10001         thee->epsz[i] = 1.0;
10002     }
10003
10004     /* Loop through the atoms and do assign the dielectric */
10005     for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
10006
10007         atom = Valist_getAtom(alist, iatom);
10008         apos = Vatom_getPosition(atom);
10009         arad = Vatom_getRadius(atom);
10010
10011         b = arad - splineWin;
10012         e = arad + splineWin;
10013         e2 = e * e;
10014         e3 = e2 * e;
10015         e4 = e3 * e;
10016         e5 = e4 * e;
10017         e6 = e5 * e;
10018         e7 = e6 * e;
10019         b2 = b * b;
10020         b3 = b2 * b;
10021         b4 = b3 * b;
10022         b5 = b4 * b;
10023         b6 = b5 * b;

```

```

10024     b7 = b6 * b;
10025     denom = e7 - 7.0*b*e6 + 21.0*b2*e5 - 35.0*e4*b3
10026             + 35.0*e3*b4 - 21.0*b5*e2 + 7.0*e*b6 - b7;
10027     c0 = b4*(35.0*e3 - 21.0*b*e2 + 7*e*b2 - b3)/denom;
10028     c1 = -140.0*b3*e3/denom;
10029     c2 = 210.0*e2*b2*(e + b)/denom;
10030     c3 = -140.0*e*b*(e2 + 3.0*b*e + b2)/denom;
10031     c4 = 35.0*(e3 + 9.0*b*e2 + 9.0*e*b2 + b3)/denom;
10032     c5 = -84.0*(e2 + 3.0*b*e + b2)/denom;
10033     c6 = 70.0*(e + b)/denom;
10034     c7 = -20.0/denom;
10035
10036     b = irad + arad - splineWin;
10037     e = irad + arad + splineWin;
10038     e2 = e * e;
10039     e3 = e2 * e;
10040     e4 = e3 * e;
10041     e5 = e4 * e;
10042     e6 = e5 * e;
10043     e7 = e6 * e;
10044     b2 = b * b;
10045     b3 = b2 * b;
10046     b4 = b3 * b;
10047     b5 = b4 * b;
10048     b6 = b5 * b;
10049     b7 = b6 * b;
10050     denom = e7 - 7.0*b*e6 + 21.0*b2*e5 - 35.0*e4*b3
10051             + 35.0*e3*b4 - 21.0*b5*e2 + 7.0*e*b6 - b7;
10052     ic0 = b4*(35.0*e3 - 21.0*b*e2 + 7*e*b2 - b3)/denom;
10053     ic1 = -140.0*b3*e3/denom;
10054     ic2 = 210.0*e2*b2*(e + b)/denom;
10055     ic3 = -140.0*e*b*(e2 + 3.0*b*e + b2)/denom;
10056     ic4 = 35.0*(e3 + 9.0*b*e2 + 9.0*e*b2 + b3)/denom;
10057     ic5 = -84.0*(e2 + 3.0*b*e + b2)/denom;
10058     ic6 = 70.0*(e + b)/denom;
10059     ic7 = -20.0/denom;
10060
10061     /* Make sure we're on the grid */
10062     if ((apos[0]<=xmin) || (apos[0]>=xmax) || \
10063         (apos[1]<=ymin) || (apos[1]>=ymax) || \
10064         (apos[2]<=zmin) || (apos[2]>=zmax)) {
10065         if ((three->pmgp->bcfl != BCFL_FOCUS) &&
10066             (three->pmgp->bcfl != BCFL_MAP)) {
10067             Vnm_print(2, "Vpmg_fillco: Atom #d at (%4.3f, %4.3f, \
10068 %4.3f) is off the mesh (ignoring):\n",
10069                     iatom, apos[0], apos[1], apos[2]);
10070             Vnm_print(2, "Vpmg_fillco:      xmin = %g, xmax = %g\n",
10071                     xmin, xmax);
10072             Vnm_print(2, "Vpmg_fillco:      ymin = %g, ymax = %g\n",
10073                     ymin, ymax);
10074             Vnm_print(2, "Vpmg_fillco:      zmin = %g, zmax = %g\n",
10075                     zmin, zmax);
10076         }
10077         fflush(stderr);
10078     } else if (arad > VPMGSMALL) { /* if we're on the mesh */
10079
10080         /* Convert the atom position to grid reference frame */
10081         position[0] = apos[0] - xmin;
10082         position[1] = apos[1] - ymin;
10083         position[2] = apos[2] - zmin;
10084
10085         /* MARK ION ACCESSIBILITY AND DIELECTRIC VALUES FOR LATER
10086          * ASSIGNMENT (Steps #1-3) */
10087         itot = irad + arad + splineWin;
10088         itot2 = VSQR(itot);
10089         ictot = VMAX2(0, (irad + arad - splineWin));
10090         ictot2 = VSQR(ictot);
10091         stot = arad + splineWin;
10092         stot2 = VSQR(stot);
10093         sctot = VMAX2(0, (arad - splineWin));
10094         sctot2 = VSQR(sctot);
10095
10096         /* We'll search over grid points which are in the greater of
10097          * these two radii */
10098         rtot = VMAX2(itot, stot);
10099         rtot2 = VMAX2(itot2, stot2);
10100         dx = rtot + 0.5*hx;
10101         dy = rtot + 0.5*hy;
10102         dz = rtot + 0.5*hzed;
10103         imin = VMAX2(0, (int)floor((position[0] - dx)/hx));
10104

```

```

10105     imax = VMIN2(nx-1, (int)ceil((position[0] + dx)/hx));
10106     jmin = VMAX2(0, (int)floor((position[1] - dy)/hy));
10107     jmax = VMIN2(ny-1, (int)ceil((position[1] + dy)/hy));
10108     kmin = VMAX2(0, (int)floor((position[2] - dz)/hzed));
10109     kmax = VMIN2(nz-1, (int)ceil((position[2] + dz)/hzed));
10110     for (i=imin; i<=imax; i++) {
10111         dx2 = VSQR(position[0] - hx*i);
10112         for (j=jmin; j<=jmax; j++) {
10113             dy2 = VSQR(position[1] - hy*j);
10114             for (k=kmin; k<=kmax; k++) {
10115                 dz2 = VSQR(position[2] - k*hzed);
10116
10117                 /* ASSIGN CCF */
10118                 if (thee->kappa[IJK(i,j,k)] > VPMGSMALL) {
10119                     dist2 = dz2 + dy2 + dx2;
10120                     if (dist2 >= itot2) {
10121                         ;
10122                     }
10123                     if (dist2 <= ictot2) {
10124                         thee->kappa[IJK(i,j,k)] = 0.0;
10125                     }
10126                     if ((dist2 < itot2) && (dist2 > ictot2)) {
10127                         dist = VSQRT(dist2);
10128                         sm = dist;
10129                         sm2 = dist2;
10130                         sm3 = sm2 * sm;
10131                         sm4 = sm3 * sm;
10132                         sm5 = sm4 * sm;
10133                         sm6 = sm5 * sm;
10134                         sm7 = sm6 * sm;
10135                         value = ic0 + ic1*sm + ic2*sm2 + ic3*sm3
10136                             + ic4*sm4 + ic5*sm5 + ic6*sm6 + ic7*sm7;
10137                         if (value > 1.0) {
10138                             value = 1.0;
10139                         } else if (value < 0.0) {
10140                             value = 0.0;
10141                         }
10142                         thee->kappa[IJK(i,j,k)] *= value;
10143                     }
10144                 }
10145
10146                 /* ASSIGN A1CF */
10147                 if (thee->epsx[IJK(i,j,k)] > VPMGSMALL) {
10148                     dist2 = dz2+dy2+VSQR(position[0]-(i+0.5)*hx);
10149                     if (dist2 >= stot2) {
10150                         thee->epsx[IJK(i,j,k)] *= 1.0;
10151                     }
10152                     if (dist2 <= sctot2) {
10153                         thee->epsx[IJK(i,j,k)] = 0.0;
10154                     }
10155                     if ((dist2 > sctot2) && (dist2 < stot2)) {
10156                         dist = VSQRT(dist2);
10157                         sm = dist;
10158                         sm2 = VSQR(sm);
10159                         sm3 = sm2 * sm;
10160                         sm4 = sm3 * sm;
10161                         sm5 = sm4 * sm;
10162                         sm6 = sm5 * sm;
10163                         sm7 = sm6 * sm;
10164                         value = c0 + c1*sm + c2*sm2 + c3*sm3
10165                             + c4*sm4 + c5*sm5 + c6*sm6 + c7*sm7;
10166                         if (value > 1.0) {
10167                             value = 1.0;
10168                         } else if (value < 0.0) {
10169                             value = 0.0;
10170                         }
10171                         thee->epsx[IJK(i,j,k)] *= value;
10172                     }
10173                 }
10174
10175                 /* ASSIGN A2CF */
10176                 if (thee->epsy[IJK(i,j,k)] > VPMGSMALL) {
10177                     dist2 = dz2+dx2+VSQR(position[1]-(j+0.5)*hy);
10178                     if (dist2 >= stot2) {
10179                         thee->epsy[IJK(i,j,k)] *= 1.0;
10180                     }
10181                     if (dist2 <= sctot2) {
10182                         thee->epsy[IJK(i,j,k)] = 0.0;
10183                     }
10184                     if ((dist2 > sctot2) && (dist2 < stot2)) {
10185                         dist = VSQRT(dist2);

```

```

10186             sm = dist;
10187             sm2 = VSQR(sm);
10188             sm3 = sm2 * sm;
10189             sm4 = sm3 * sm;
10190             sm5 = sm4 * sm;
10191             sm6 = sm5 * sm;
10192             sm7 = sm6 * sm;
10193             value = c0 + c1*sm + c2*sm2 + c3*sm3
10194                   + c4*sm4 + c5*sm5 + c6*sm6 + c7*sm7;
10195             if (value > 1.0) {
10196                 value = 1.0;
10197             } else if (value < 0.0) {
10198                 value = 0.0;
10199             }
10200             thee->epsy[IJK(i,j,k)] *= value;
10201         }
10202     }
10203
10204     /* ASSIGN A3CF */
10205     if (thee->epsz[IJK(i,j,k)] > VPMGSMALL) {
10206         dist2 = dy2+dx2+VSQR(position[2]-(k+0.5)*hzd);
10207         if (dist2 >= stot2) {
10208             thee->epsz[IJK(i,j,k)] *= 1.0;
10209         }
10210         if (dist2 <= sctot2) {
10211             thee->epsz[IJK(i,j,k)] = 0.0;
10212         }
10213         if ((dist2 > sctot2) && (dist2 < stot2)) {
10214             dist = VSQRT(dist2);
10215             sm = dist;
10216             sm2 = dist2;
10217             sm3 = sm2 * sm;
10218             sm4 = sm3 * sm;
10219             sm5 = sm4 * sm;
10220             sm6 = sm5 * sm;
10221             sm7 = sm6 * sm;
10222             value = c0 + c1*sm + c2*sm2 + c3*sm3
10223                   + c4*sm4 + c5*sm5 + c6*sm6 + c7*sm7;
10224             if (value > 1.0) {
10225                 value = 1.0;
10226             } else if (value < 0.0) {
10227                 value = 0.0;
10228             }
10229             thee->epsz[IJK(i,j,k)] *= value;
10230         }
10231     }
10232
10233     } /* k loop */
10234 } /* j loop */
10235 } /* i loop */
10236 } /* endif (on the mesh) */
10237 } /* endfor (over all atoms) */
10238
10239 Vnm_print(0, "Vpmg_fillco: filling coefficient arrays\n");
10240 /* Interpret markings and fill the coefficient arrays */
10241 for (k=0; k<nz; k++) {
10242     for (j=0; j<ny; j++) {
10243         for (i=0; i<nx; i++) {
10244
10245             thee->kappa[IJK(i,j,k)] = ionmask*thee->kappa[IJK(i,j,k)];
10246             thee->epsx[IJK(i,j,k)] = (epsw-epsp)*thee->epsx[IJK(i,j,k)]
10247                 + epsp;
10248             thee->epsy[IJK(i,j,k)] = (epsw-epsp)*thee->epsy[IJK(i,j,k)]
10249                 + epsp;
10250             thee->epsz[IJK(i,j,k)] = (epsw-epsp)*thee->epsz[IJK(i,j,k)]
10251                 + epsp;
10252
10253         } /* i loop */
10254     } /* j loop */
10255 } /* k loop */
10256 }
10257
10258 }
10259
10260 VPUBLIC void fillcoPermanentInduced(Vpmg *thee) {
10261
10262     Valist *alist;
10263     Vpbe *pbe;
10264     Vatom *atom;
10265     /* Coverisions */
10266     double zmagic, f;

```

```

10267  /* Grid */
10268  double xmin, xmax, ymin, ymax, zmin, zmax;
10269  double xlen, ylen, zlen, position[3], ifloat, jfloat, kfloat;
10270  double hx, hy, hzed, *apos;
10271  /* Multipole */
10272  double charge, *dipole, *quad;
10273  double c, ux, uy, uz, qxx, qyx, qyy, qzx, qzy, qzz, qave;
10274  /* B-spline weights */
10275  double mx, my, mz, dmx, dmy, dmz, d2mx, d2my, d2mz;
10276  double mi, mj, mk;
10277  /* Loop variables */
10278  int i, ii, jj, kk, nx, ny, nz, iatom;
10279  int im2, im1, ip1, ip2, jm2, jm1, jp1, jp2, km2, km1, kp1, kp2;
10280
10281  VASSERT(thee != VNULL);
10282
10283  /* Get PBE info */
10284  pbe = thee->pbe;
10285  alist = pbe->alist;
10286  zmagic = Vpbe_getZmagic(pbe);
10287
10288  /* Mesh info */
10289  nx = thee->pmgp->nx;
10290  ny = thee->pmgp->ny;
10291  nz = thee->pmgp->nz;
10292  hx = thee->pmgp->hx;
10293  hy = thee->pmgp->hy;
10294  hzed = thee->pmgp->hzed;
10295
10296  /* Conversion */
10297  f = zmagic/(hx*hy*hzed);
10298
10299  /* Define the total domain size */
10300  xlen = thee->pmgp->xlen;
10301  ylen = thee->pmgp->ylen;
10302  zlen = thee->pmgp->zlen;
10303
10304  /* Define the min/max dimensions */
10305  xmin = thee->pmgp->xcent - (xlen/2.0);
10306  ymin = thee->pmgp->ycent - (ylen/2.0);
10307  zmin = thee->pmgp->zcent - (zlen/2.0);
10308  xmax = thee->pmgp->xcent + (xlen/2.0);
10309  ymax = thee->pmgp->ycent + (ylen/2.0);
10310  zmax = thee->pmgp->zcent + (zlen/2.0);
10311
10312  /* Fill in the source term (permanent atomic multipoles
10313   and induced dipoles) */
10314  Vnm_print(0, "fillCoPermanentInduced: filling in source term.\n");
10315  for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
10316
10317      atom = Valist_getAtom(alist, iatom);
10318      apos = Vatom_getPosition(atom);
10319
10320      c = Vatom_getCharge(atom)*f;
10321
10322      #if defined(WITH_TINKER)
10323          dipole = Vatom_getDipole(atom);
10324          ux = dipole[0]/hx*f;
10325          uy = dipole[1]/hy*f;
10326          uz = dipole[2]/hzed*f;
10327          dipole = Vatom_getInducedDipole(atom);
10328          ux = ux + dipole[0]/hx*f;
10329          uy = uy + dipole[1]/hy*f;
10330          uz = uz + dipole[2]/hzed*f;
10331          quad = Vatom_getQuadrupole(atom);
10332          qxx = (1.0/3.0)*quad[0]/(hx*hx)*f;
10333          qyx = (2.0/3.0)*quad[3]/(hx*hy)*f;
10334          qyy = (1.0/3.0)*quad[4]/(hy*hy)*f;
10335          qzx = (2.0/3.0)*quad[6]/(hzed*hx)*f;
10336          qzy = (2.0/3.0)*quad[7]/(hzed*hy)*f;
10337          qzz = (1.0/3.0)*quad[8]/(hzed*hzed)*f;
10338      #else
10339          ux = 0.0;
10340          uy = 0.0;
10341          uz = 0.0;
10342          qxx = 0.0;
10343          qyx = 0.0;
10344          qyy = 0.0;
10345          qzx = 0.0;
10346          qzy = 0.0;
10347          qzz = 0.0;

```

```

10348 #endif /* if defined(WITH_TINKER) */
10349
10350     /* Make sure we're on the grid */
10351     if ((apos[0]<=(xmin-2*hx)) || (apos[0]>=(xmax+2*hx)) || \
10352         (apos[1]<=(ymin-2*hy)) || (apos[1]>=(ymax+2*hy)) || \
10353         (apos[2]<=(zmin-2*hzed)) || (apos[2]>=(zmax+2*hzed))) {
10354         Vnm_print(2, "fillcoPermanentMultipole: Atom #\n", iatom, apos[0], apos[1], apos[2]);
10355         (ignoring this atom):\n";
10356         Vnm_print(2, "fillcoPermanentMultipole: xmin = %g, xmax = %g\n", xmin, xmax);
10357         Vnm_print(2, "fillcoPermanentMultipole: ymin = %g, ymax = %g\n", ymin, ymax);
10358         Vnm_print(2, "fillcoPermanentMultipole: zmin = %g, zmax = %g\n", zmin, zmax);
10359         fflush(stderr);
10360     } else {
10361         /* Convert the atom position to grid reference frame */
10362         position[0] = apos[0] - xmin;
10363         position[1] = apos[1] - ymin;
10364         position[2] = apos[2] - zmin;
10365
10366         /* Figure out which vertices we're next to */
10367         ifloat = position[0]/hx;
10368         jfloat = position[1]/hy;
10369         kfloat = position[2]/hzed;
10370
10371         ip1 = (int)ceil(ifloat);
10372         ip2 = ip1 + 2;
10373         im1 = (int)floor(ifloat);
10374         im2 = im1 - 2;
10375         jp1 = (int)ceil(jfloat);
10376         jp2 = jp1 + 2;
10377         jm1 = (int)floor(jfloat);
10378         jm2 = jm1 - 2;
10379         kp1 = (int)ceil(kfloat);
10380         kp2 = kp1 + 2;
10381         km1 = (int)floor(kfloat);
10382         km2 = km1 - 2;
10383
10384         /* This step shouldn't be necessary, but it saves nasty debugging
10385          * later on if something goes wrong */
10386         ip2 = VMIN2(ip2,nx-1);
10387         ip1 = VMIN2(ip1,nx-1);
10388         im1 = VMAX2(im1,0);
10389         im2 = VMAX2(im2,0);
10390         jp2 = VMIN2(jp2,ny-1);
10391         jp1 = VMIN2(jp1,ny-1);
10392         jm1 = VMAX2(jm1,0);
10393         jm2 = VMAX2(jm2,0);
10394         kp2 = VMIN2(kp2,nz-1);
10395         kp1 = VMIN2(kp1,nz-1);
10396         km1 = VMAX2(km1,0);
10397         km2 = VMAX2(km2,0);
10398
10399         /* Now assign fractions of the charge to the nearby verts */
10400         for (ii=im2; ii<=ip2; ii++) {
10401             mi = VFCHI4(ii,ifloat);
10402             mx = bspline4(mi);
10403             dm1 = dbspline4(mi);
10404             d2m1 = d2bspline4(mi);
10405             for (jj=jm2; jj<=jp2; jj++) {
10406                 mj = VFCHI4(jj,jfloat);
10407                 my = bspline4(mj);
10408                 dmy = dbspline4(mj);
10409                 d2my = d2bspline4(mj);
10410                 for (kk=km2; kk<=kp2; kk++) {
10411                     mk = VFCHI4(kk,kfloat);
10412                     mz = bspline4(mk);
10413                     dmz = dbspline4(mk);
10414                     d2mz = d2bspline4(mk);
10415                     charge = mx*my*mz*c -
10416                         dm1*my*mz*ux - mx*dmy*mz*uy - mx*my*dmy*uz +
10417                         d2m1*my*mz*qxx +
10418                         dm1*dmy*mz*qyx + mx*d2my*mz*qyy +
10419                         dm1*my*dmy*qzx + mx*dmy*dmy*qzy + mx*my*d2mz*qzz;
10420                     thee->charge[IJK(ii,jj,kk)] += charge;
10421                 }
10422             }
10423         }
10424     } /* endif (on the mesh) */
10425 } /* endfor (each atom) */
10426
10427

```

```

10428 }
10429
10430 VPRIVATE void fillCoefSpline3(Vpmg *thee) {
10431     Valist *alist;
10432     Vpbe *pbe;
10433     Vatom *atom;
10434     double xmin, xmax, ymin, ymax, zmin, zmax, ionmask, ionstr, dist2;
10435     double xlen, ylen, zlen, position[3], itot, stot, ictot, ictot2, sctot;
10436     double irad, dx, dy, dz, epsw, epsp, w2i;
10437     double hx, hy, hzed, *apos, arad, sctot2;
10438     double dx2, dy2, dz2, stot2, itot2, rtot, rtot2, splineWin;
10439     double dist, value, denom, sm, sm2, sm3, sm4, sm5;
10440     double e, e2, e3, e4, e5;
10441     double b, b2, b3, b4, b5;
10442     double c0, c1, c2, c3, c4, c5;
10443     double ic0, ic1, ic2, ic3, ic4, ic5;
10444     int i, j, k, nx, ny, nz, iatom;
10445     int imin, imax, jmin, jmax, kmin, kmax;
10446
10447     VASSERT(thee != VNULL);
10448     splineWin = thee->splineWin;
10449
10450     /* Get PBE info */
10451     pbe = thee->pbe;
10452     alist = pbe->alist;
10453     irad = Vpbe_getMaxIonRadius(pbe);
10454     ionstr = Vpbe_getBulkIonicStrength(pbe);
10455     epsw = Vpbe_getSolventDiel(pbe);
10456     epsp = Vpbe_getSoluteDiel(pbe);
10457
10458     /* Mesh info */
10459     nx = thee->pmgp->nx;
10460     ny = thee->pmgp->ny;
10461     nz = thee->pmgp->nz;
10462     hx = thee->pmgp->hx;
10463     hy = thee->pmgp->hy;
10464     hzed = thee->pmgp->hzed;
10465
10466     /* Define the total domain size */
10467     xlen = thee->pmgp->xlen;
10468     ylen = thee->pmgp->ylen;
10469     zlen = thee->pmgp->zlen;
10470
10471     /* Define the min/max dimensions */
10472     xmin = thee->pmgp->xcent - (xlen/2.0);
10473     ymin = thee->pmgp->ycent - (ylen/2.0);
10474     zmin = thee->pmgp->zcent - (zlen/2.0);
10475     xmax = thee->pmgp->xcent + (xlen/2.0);
10476     ymax = thee->pmgp->ycent + (ylen/2.0);
10477     zmax = thee->pmgp->zcent + (zlen/2.0);
10478
10479     /* This is a floating point parameter related to the non-zero nature of the
10480      * bulk ionic strength. If the ionic strength is greater than zero; this
10481      * parameter is set to 1.0 and later scaled by the appropriate pre-factors.
10482      * Otherwise, this parameter is set to 0.0 */
10483     if (ionstr > VPMGSMALL) ionmask = 1.0;
10484     else ionmask = 0.0;
10485
10486     /* Reset the kappa, epsx, epsy, and epsz arrays */
10487     for (i=0; i<(nx*ny*nz); i++) {
10488         thee->kappa[i] = 1.0;
10489         thee->epsx[i] = 1.0;
10490         thee->epsy[i] = 1.0;
10491         thee->epsz[i] = 1.0;
10492     }
10493
10494     /* Loop through the atoms and do assign the dielectric */
10495     for (iatom=0; iatom<Valist_getNumberAtoms(alist); iatom++) {
10496         atom = Valist_getAtom(alist, iatom);
10497         apos = Vatom_getPosition(atom);
10498         arad = Vatom_getRadius(atom);
10499
10500         b = arad - splineWin;
10501         e = arad + splineWin;
10502         e2 = e * e;
10503         e3 = e2 * e;
10504         e4 = e3 * e;
10505         e5 = e4 * e;
10506         b2 = b * b;

```

```

10509      b3 = b2 * b;
10510      b4 = b3 * b;
10511      b5 = b4 * b;
10512      denom = pow((e - b), 5.0);
10513      c0 = -10.0*e2*b3 + 5.0*e*b4 - b5;
10514      c1 = 30.0*e2*b2;
10515      c2 = -30.0*(e2*b + e*b2);
10516      c3 = 10.0*(e2 + 4.0*e*b + b2);
10517      c4 = -15.0*(e + b);
10518      c5 = 6;
10519      c0 = c0/denom;
10520      c1 = c1/denom;
10521      c2 = c2/denom;
10522      c3 = c3/denom;
10523      c4 = c4/denom;
10524      c5 = c5/denom;
10525
10526      b = irad + arad - splineWin;
10527      e = irad + arad + splineWin;
10528      e2 = e * e;
10529      e3 = e2 * e;
10530      e4 = e3 * e;
10531      e5 = e4 * e;
10532      b2 = b * b;
10533      b3 = b2 * b;
10534      b4 = b3 * b;
10535      b5 = b4 * b;
10536      denom = pow((e - b), 5.0);
10537      ic0 = -10.0*e2*b3 + 5.0*e*b4 - b5;
10538      ic1 = 30.0*e2*b2;
10539      ic2 = -30.0*(e2*b + e*b2);
10540      ic3 = 10.0*(e2 + 4.0*e*b + b2);
10541      ic4 = -15.0*(e + b);
10542      ic5 = 6;
10543      ic0 = c0/denom;
10544      ic1 = c1/denom;
10545      ic2 = c2/denom;
10546      ic3 = c3/denom;
10547      ic4 = c4/denom;
10548      ic5 = c5/denom;
10549
10550      /* Make sure we're on the grid */
10551      if ((apos[0]<=xmin) || (apos[0]>=xmax) || \
10552          (apos[1]<=ymin) || (apos[1]>=ymax) || \
10553          (apos[2]<=zmin) || (apos[2]>=zmax)) {
10554          if ((three->pmgp->bcfl != BCFL_FOCUS) &&
10555              (three->pmgp->bcfl != BCFL_MAP)) {
10556              Vnm_print(2, "Vpmg_fillco: Atom #d at (%4.3f, %4.3f,\
10557 %4.3f) is off the mesh (ignoring):\n",
10558                      iatom, apos[0], apos[1], apos[2]);
10559              Vnm_print(2, "Vpmg_fillco:      xmin = %g, xmax = %g\n",
10560                      xmin, xmax);
10561              Vnm_print(2, "Vpmg_fillco:      ymin = %g, ymax = %g\n",
10562                      ymin, ymax);
10563              Vnm_print(2, "Vpmg_fillco:      zmin = %g, zmax = %g\n",
10564                      zmin, zmax);
10565          }
10566          fflush(stderr);
10567
10568      } else if (arad > VPMGSMALL) { /* if we're on the mesh */
10569
10570          /* Convert the atom position to grid reference frame */
10571          position[0] = apos[0] - xmin;
10572          position[1] = apos[1] - ymin;
10573          position[2] = apos[2] - zmin;
10574
10575          /* MARK ION ACCESSIBILITY AND DIELECTRIC VALUES FOR LATER
10576           * ASSIGNMENT (Steps #1-3) */
10577          itot = irad + arad + splineWin;
10578          itot2 = VSQR(itot);
10579          ictot = VMAX2(0, (irad + arad - splineWin));
10580          ictot2 = VSQR(ictot);
10581          stot = arad + splineWin;
10582          stot2 = VSQR(stot);
10583          sctot = VMAX2(0, (arad - splineWin));
10584          sctot2 = VSQR(sctot);
10585
10586          /* We'll search over grid points which are in the greater of
10587           * these two radii */
10588          rtot = VMAX2(itot, stot);
10589          rtot2 = VMAX2(itot2, stot2);

```



```

10590     dx = rtot + 0.5*hx;
10591     dy = rtot + 0.5*hy;
10592     dz = rtot + 0.5*hzed;
10593     imin = VMAX2(0, (int)floor((position[0] - dx)/hx));
10594     imax = VMIN2(nx-1, (int)ceil((position[0] + dx)/hx));
10595     jmin = VMAX2(0, (int)floor((position[1] - dy)/hy));
10596     jmax = VMIN2(ny-1, (int)ceil((position[1] + dy)/hy));
10597     kmin = VMAX2(0, (int)floor((position[2] - dz)/hzed));
10598     kmax = VMIN2(nz-1, (int)ceil((position[2] + dz)/hzed));
10599     for (i=imin; i<=imax; i++) {
10600         dx2 = VSQR(position[0] - hx*i);
10601         for (j=jmin; j<=jmax; j++) {
10602             dy2 = VSQR(position[1] - hy*j);
10603             for (k=kmin; k<=kmax; k++) {
10604                 dz2 = VSQR(position[2] - k*hzed);
10605
10606                 /* ASSIGN CCF */
10607                 if (thee->kappa[IJK(i,j,k)] > VPMGSMALL) {
10608                     dist2 = dz2 + dy2 + dx2;
10609                     if (dist2 >= itot2) {
10610                         ;
10611                     }
10612                     if (dist2 <= ictot2) {
10613                         thee->kappa[IJK(i,j,k)] = 0.0;
10614                     }
10615                     if ((dist2 < itot2) && (dist2 > ictot2)) {
10616                         dist = VSQRT(dist2);
10617                         sm = dist;
10618                         sm2 = dist2;
10619                         sm3 = sm2 * sm;
10620                         sm4 = sm3 * sm;
10621                         sm5 = sm4 * sm;
10622                         value = ic0 + ic1*sm + ic2*sm2 + ic3*sm3
10623                             + ic4*sm4 + ic5*sm5;
10624                         if (value > 1.0) {
10625                             value = 1.0;
10626                         } else if (value < 0.0) {
10627                             value = 0.0;
10628                         }
10629                         thee->kappa[IJK(i,j,k)] *= value;
10630                     }
10631                 }
10632
10633                 /* ASSIGN A1CF */
10634                 if (thee->epsx[IJK(i,j,k)] > VPMGSMALL) {
10635                     dist2 = dz2+dy2+VSQR(position[0]-(i+0.5)*hx);
10636                     if (dist2 >= stot2) {
10637                         thee->epsx[IJK(i,j,k)] *= 1.0;
10638                     }
10639                     if (dist2 <= sctot2) {
10640                         thee->epsx[IJK(i,j,k)] = 0.0;
10641                     }
10642                     if ((dist2 > sctot2) && (dist2 < stot2)) {
10643                         dist = VSQRT(dist2);
10644                         sm = dist;
10645                         sm2 = VSQR(sm);
10646                         sm3 = sm2 * sm;
10647                         sm4 = sm3 * sm;
10648                         sm5 = sm4 * sm;
10649                         value = c0 + c1*sm + c2*sm2 + c3*sm3
10650                             + c4*sm4 + c5*sm5;
10651                         if (value > 1.0) {
10652                             value = 1.0;
10653                         } else if (value < 0.0) {
10654                             value = 0.0;
10655                         }
10656                         thee->epsx[IJK(i,j,k)] *= value;
10657                     }
10658                 }
10659
10660                 /* ASSIGN A2CF */
10661                 if (thee->epsy[IJK(i,j,k)] > VPMGSMALL) {
10662                     dist2 = dz2+dx2+VSQR(position[1]-(j+0.5)*hy);
10663                     if (dist2 >= stot2) {
10664                         thee->epsy[IJK(i,j,k)] *= 1.0;
10665                     }
10666                     if (dist2 <= sctot2) {
10667                         thee->epsy[IJK(i,j,k)] = 0.0;
10668                     }
10669                     if ((dist2 > sctot2) && (dist2 < stot2)) {
10670                         dist = VSQRT(dist2);

```

```

10671         sm = dist;
10672         sm2 = VSQR(sm);
10673         sm3 = sm2 * sm;
10674         sm4 = sm3 * sm;
10675         sm5 = sm4 * sm;
10676         value = c0 + c1*sm + c2*sm2 + c3*sm3
10677             + c4*sm4 + c5*sm5;
10678         if (value > 1.0) {
10679             value = 1.0;
10680         } else if (value < 0.0) {
10681             value = 0.0;
10682         }
10683         thee->epsy[IJK(i,j,k)] *= value;
10684     }
10685 }
10686
10687 /* ASSIGN A3CF */
10688 if (thee->epsz[IJK(i,j,k)] > VPMGSMALL) {
10689     dist2 = dy2+dx2+VSQR(position[2]-(k+0.5)*hzd);
10690     if (dist2 >= stot2) {
10691         thee->epsz[IJK(i,j,k)] *= 1.0;
10692     }
10693     if (dist2 <= sctot2) {
10694         thee->epsz[IJK(i,j,k)] = 0.0;
10695     }
10696     if ((dist2 > sctot2) && (dist2 < stot2)) {
10697         dist = VSQRT(dist2);
10698         sm = dist;
10699         sm2 = dist2;
10700         sm3 = sm2 * sm;
10701         sm4 = sm3 * sm;
10702         sm5 = sm4 * sm;
10703         value = c0 + c1*sm + c2*sm2 + c3*sm3
10704             + c4*sm4 + c5*sm5;
10705         if (value > 1.0) {
10706             value = 1.0;
10707         } else if (value < 0.0) {
10708             value = 0.0;
10709         }
10710         thee->epsz[IJK(i,j,k)] *= value;
10711     }
10712 }
10713
10714     } /* k loop */
10715 } /* j loop */
10716 } /* i loop */
10717 } /* endif (on the mesh) */
10718 } /* endfor (over all atoms) */
10719
10720 Vnm_print(0, "Vpmg_fillco: filling coefficient arrays\n");
10721 /* Interpret markings and fill the coefficient arrays */
10722 for (k=0; k<nz; k++) {
10723     for (j=0; j<ny; j++) {
10724         for (i=0; i<nx; i++) {
10725
10726             thee->kappa[IJK(i,j,k)] = ionmask*thee->kappa[IJK(i,j,k)];
10727             thee->epsx[IJK(i,j,k)] = (epsw-epsp)*thee->epsx[IJK(i,j,k)]
10728                 + epsp;
10729             thee->epsy[IJK(i,j,k)] = (epsw-epsp)*thee->epsy[IJK(i,j,k)]
10730                 + epsp;
10731             thee->epsz[IJK(i,j,k)] = (epsw-epsp)*thee->epsz[IJK(i,j,k)]
10732                 + epsp;
10733
10734         } /* i loop */
10735     } /* j loop */
10736 } /* k loop */
10737
10738 }
10739
10740
10741 VPRIVATE void bcolcomp(int *iparm, double *rparm, int *iwork, double *rwork,
10742     double *values, int *rowind, int *colptr, int *flag) {
10743     int nrow, ncol, nnzero, i;
10744     int nxc, nyc, nzc, nf, nc, narr, narrc, n_rpc;
10745     int n_iz, n_ipc, iretot, iintot;
10746     int nrwk, niwk, nx, ny, nz, nlev, ierror, maxlev, mxlv;
10747     int mgcoar, mgdisc, mgsolv;
10748     int k_iz;
10749     int k_ipc, k_rpc, k_ac, k_cc, k_fc, k_pc;
10750
10751     WARN_UNTESTED;

```

```

10752
10753 // Decode some parameters
10754 nrwk = VAT(iparm, 1);
10755 niwk = VAT(iparm, 2);
10756 nx   = VAT(iparm, 3);
10757 ny   = VAT(iparm, 4);
10758 nz   = VAT(iparm, 5);
10759 nlev = VAT(iparm, 6);
10760
10761 // Some checks on input
10762 mxlv = Vmaxlev(nx, ny, nz);
10763
10764 // Basic grid sizes, etc.
10765 mgcoar = VAT(iparm, 18);
10766 mgdisc = VAT(iparm, 19);
10767 mgsolv = VAT(iparm, 21);
10768 Vmgisz(&mgcoar, &mgdisc, &mgsolv,
10769        &nx, &ny, &nz,
10770        &nlev,
10771        &nxc, &nyc, &nzc,
10772        &nf, &nc,
10773        &narr, &narrc,
10774        &n_rpc, &n_iz, &n_ipc,
10775        &ioretot, &iintot);
10776
10777 // Split up the integer work array
10778 k_iz = 1;
10779 k_ipc = k_iz + n_iz;
10780
10781 // Split up the real work array
10782 k_rpc = 1;
10783 k_cc  = k_rpc + n_rpc;
10784 k_fc  = k_cc  + narr;
10785 k_pc  = k_fc  + narr;
10786 k_ac  = k_pc  + 27*narrc;
10787
10788 bcolcomp2(iparm, rparm,
10789            &nx, &ny, &nz, RAT(iwork, k_iz),
10790            RAT(iwork, k_ipc), RAT(rwork, k_rpc),
10791            RAT(rwork, k_ac), RAT(rwork, k_cc),
10792            values, rowind, colptr, flag);
10793 }
10794
10795 VPRIVATE void bcolcomp2(int *iparm, double *rparm,
10796                          int *nx, int *ny, int *nz,
10797                          int *iz, int *ipc, double *rpc,
10798                          double *ac, double *cc, double *values,
10799                          int *rowind, int *colptr, int *flag) {
10800
10801     int nlev = 1;
10802     int lev = VAT(iparm, 6);
10803
10804     MAT2(iz, 50, nlev);
10805
10806     WARN_UNTESTED;
10807
10808     /*
10809     * Build the multigrid data structure in iz
10810     * THIS MAY HAVE BEEN DONE ALREADY, BUT IT'S OK TO DO IT AGAIN,
10811     * RIGHT?
10812     * call buildstr (nx,ny,nz,nlev,iz)
10813     *
10814     * We're interested in the finest level
10815     */
10816     bcolcomp3(nx, ny, nz,
10817               RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
10818               RAT(ac, VAT2(iz, 7, lev)), RAT(cc, VAT2(iz, 1, lev)),
10819               values, rowind, colptr, flag);
10820 }
10821
10822 /*****
10823 * Routine:  bcolcomp3
10824 * Purpose:  Build a column-compressed matrix in Harwell-Boeing format
10825 * Args:     flag  0 ==> Use Poisson operator only
10826 *           1 ==> Use linearization of full operator around current
10827 *            solution
10828 * Author:   Nathan Baker (mostly ripped off from Harwell-Boeing format
10829 *            documentation)
10830 *****/
10831 VPRIVATE void bcolcomp3(int *nx, int *ny, int *nz,
10832                          int *ipc, double *rpc,

```

```

10833     double *ac, double *cc,
10834     double *values, int *rowind, int *colptr, int *flag) {
10835
10836     MAT2(ac, *nx * *ny * *nz, 1);
10837
10838     WARN_UNTESTED;
10839
10840     bcolcomp4(nx, ny, nz,
10841             ipc, rpc,
10842             RAT2(ac, 1, 1), cc,
10843             RAT2(ac, 1, 2), RAT2(ac, 1, 3), RAT2(ac, 1, 4),
10844             values, rowind, colptr, flag);
10845 }
10846
10847
10848
10849 /*****
10850  * Routine:  bcolcomp4
10851  * Purpose:  Build a column-compressed matrix in Harwell-Boeing format
10852  * Args:     flag    0 ==> Use Poisson operator only
10853  *           1 ==> Use linearization of full operator around current
10854  *             solution
10855  * Author:    Nathan Baker (mostly ripped off from Harwell-Boeing format
10856  *             documentation)
10857  *****/
10858 PRIVATE void bcolcomp4(int *nx, int *ny, int *nz,
10859     int *ipc, double *rpc,
10860     double *oC, double *cc, double *oE, double *oN, double *uC,
10861     double *values, int *rowind, int *colptr, int *flag) {
10862
10863     int nxm2, nym2, nzm2;
10864     int ii, jj, kk, ll;
10865     int i, j, k, l;
10866     int inonz, irow, nn, nrow, ncol, nonz, irow, n;
10867
10868     int doit;
10869
10870     MAT3(oE, *nx, *ny, *nz);
10871     MAT3(oN, *nx, *ny, *nz);
10872     MAT3(uC, *nx, *ny, *nz);
10873     MAT3(cc, *nx, *ny, *nz);
10874     MAT3(oC, *nx, *ny, *nz);
10875
10876     WARN_UNTESTED;
10877
10878     // Get some column, row, and nonzero information
10879     n = *nx * *ny * *nz;
10880     nxm2 = *nx - 2;
10881     nym2 = *ny - 2;
10882     nzm2 = *nz - 2;
10883     nn = nxm2 * nym2 * nzm2;
10884     ncol = nn;
10885     nrow = nn;
10886     nonz = 7 * nn - 2 * nxm2 * nym2 - 2 * nxm2 - 2;
10887
10888     // Intialize some pointers
10889     inonz = 1;
10890
10891     /*
10892     * Run over the dimensions of the matrix (non-zero only in the interior
10893     * of the mesh
10894     */
10895     for (k=2; k<=*nz-1; k++) {
10896         // Offset the index to the output grid index
10897         kk = k - 1;
10898
10899         for (j=2; j<=*ny-1; j++) {
10900             // Offset the index to the output grid index
10901             jj = j - 1;
10902
10903             for (i=2; i<=*nx-1; i++) {
10904                 // Offset the index to the output grid index
10905                 ii = i - 1;
10906
10907                 // Get the output (i,j,k) row number in natural ordering
10908                 ll = (kk - 1) * nxm2 * nym2 + (jj - 1) * nxm2 + (ii - 1) + 1;
10909                 l = (k - 1) * *nx * *ny + (j - 1) * *nx + (i - 1) + 1;
10910
10911                 // Store where this column starts
10912                 VAT(colptr,ll) = inonz;
10913

```

```

10914         // SUB-DIAGONAL 3
10915         irow = ll - nxm2 * nym2;
10916         irow = 1 - *nx * *ny;
10917
10918         doit = (irow >= 1) && (irow <= nn);
10919         doit = doit && (irow >= 1) && (irow <= n);
10920
10921         if (doit) {
10922             VAT(values, inonz) = -VAT3(uC, i, j, k-1);
10923             VAT(rowind, inonz) = irow;
10924             inonz++;
10925         }
10926
10927
10928         // SUB-DIAGONAL 2
10929         irow = ll - nxm2;
10930         irow = 1 - *nx;
10931
10932         doit = (irow >= 1) && (irow <= nn);
10933         doit = doit && (irow >= 1) && (irow <= n);
10934
10935         if (doit) {
10936             VAT(values, inonz) = -VAT3(oN, i, j-1, k);
10937             VAT(rowind, inonz) = irow;
10938             inonz++;
10939         }
10940
10941
10942         // SUB-DIAGONAL 1
10943         irow = ll - 1;
10944         irow = 1 - 1;
10945
10946         doit = (irow >= 1) && (irow <= nn);
10947         doit = doit && (irow <= 1) && (irow <= n);
10948
10949         if (doit) {
10950             VAT(values, inonz) = -VAT3(oE, i-1, j, k);
10951             VAT(rowind, inonz) = irow;
10952             inonz++;
10953         }
10954
10955
10956         // DIAGONAL
10957         irow = ll;
10958         irow = 1;
10959
10960         if (*flag == 0) {
10961             VAT(values, inonz) = VAT3(oC, i, j, k);
10962         } else if (*flag == 1) {
10963             VAT(values, inonz) = VAT3(oC, i, j, k)
10964                             + VAT3(cc, i, j, k);
10965         } else {
10966             VABORT_MSG0("PMGF1");
10967         }
10968
10969         VAT(rowind, inonz) = irow;
10970         inonz++;
10971
10972         // SUPER-DIAGONAL 1
10973         irow = ll + 1;
10974         irow = 1 + 1;
10975         doit = (irow >= 1) && (irow <= nn);
10976         doit = doit && (irow >= 1) && (irow <= n);
10977
10978         if (doit) {
10979             VAT(values, inonz) = -VAT3(oE, i, j, k);
10980             VAT(rowind, inonz) = irow;
10981             inonz++;
10982         }
10983
10984
10985         // SUPER-DIAGONAL 2
10986         irow = ll + nxm2;
10987         irow = 1 + *nx;
10988         doit = (irow >= 1) && (irow <= nn);
10989         doit = doit && (irow >= 1) && (irow <= n);
10990
10991         if (doit) {
10992             VAT(values, inonz) = -VAT3(oN, i, j, k);
10993             VAT(rowind, inonz) = irow;
10994         }

```

```

10995             inonz++;
10996         }
10997
10998
10999
11000         // SUPER-DIAGONAL 3
11001         iirow = ll + nxm2 * nym2;
11002         irow = 1 + nx * ny;
11003         doit = (iirow >= 1) && (iirow <= nn);
11004         doit = doit && (irow >= 1) && (irow <= n);
11005         if (doit) {
11006             VAT(values, inonz) = -VAT3(uC, i, j, k);
11007             VAT(rowind, inonz) = iirow;
11008             inonz++;
11009         }
11010     }
11011 }
11012 }
11013
11014 VAT(colptr, ncol + 1) = inonz;
11015
11016 if (inonz != (nonz + 1)) {
11017     VABORT_MSG2("BCOLCOMP4: ERROR -- INONZ = %d, NONZ = %d", inonz, nonz);
11018 }
11019 }
11020
11021
11022
11023 VPRIVATE void pcolcomp(int *nrow, int *ncol, int *nnzero,
11024     double *values, int *rowind, int *colptr,
11025     char *path, char *title, char *mxttype) {
11026
11027     char key[] = "key";
11028     char ptrfmt[] = "(10I8)";
11029     char indfmt[] = "(10I8)";
11030     char valfmt[] = "(5E15.8)";
11031     char rhsfmt[] = "(5E15.8)";
11032
11033     int i, totcrd, ptrcrd, indcrd, valcrd, neltvl, rhscrd;
11034
11035     FILE *outFile;
11036
11037     WARN_UNTESTED;
11038
11039     // Open the file for reading
11040     outFile = fopen(path, "w");
11041
11042     // Set some default values
11043     ptrcrd = (int)(*ncol / 10 + 1) - 1;
11044     indcrd = (int)(*nnzero / 10 + 1) - 1;
11045     valcrd = (int)(*nnzero / 10 + 1) - 1;
11046     totcrd = ptrcrd + indcrd + valcrd;
11047     rhscrd = 0;
11048     neltvl = 0;
11049
11050     // Print the header
11051     fprintf(outFile, "%72s%8s\n",
11052         title, key);
11053     fprintf(outFile, "%14d%14d%14d%14d%14d\n",
11054         totcrd, ptrcrd, indcrd, valcrd, rhscrd);
11055     fprintf(outFile, "%3s\n", mxttype);
11056     fprintf(outFile, "%14d%14d%14d%14d\n",
11057         *nrow, *ncol, *nnzero, neltvl);
11058     fprintf(outFile, "%16s%16s%20s%20s\n",
11059         ptrfmt, indfmt, valfmt, rhsfmt);
11060
11061     // Write the matrix structure
11062     for (i=1; i<=*ncol+1; i++)
11063         fprintf(outFile, "%8d", VAT(colptr, i));
11064     fprintf(outFile, "\n");
11065
11066     for (i=1; i<=*nnzero; i++)
11067         fprintf(outFile, "%8d", VAT(rowind, i));
11068     fprintf(outFile, "\n");
11069
11070     // Write out the values
11071     if (valcrd > 0) {
11072         for (i=1; i<=*nnzero; i++)
11073             fprintf(outFile, "%15.8e", VAT(values, i));
11074         fprintf(outFile, "\n");
11075     }

```

```
11076
11077     // Close the file
11078     fclose (outFile);
11079 }
```

9.108 src/mg/vpmg.h File Reference

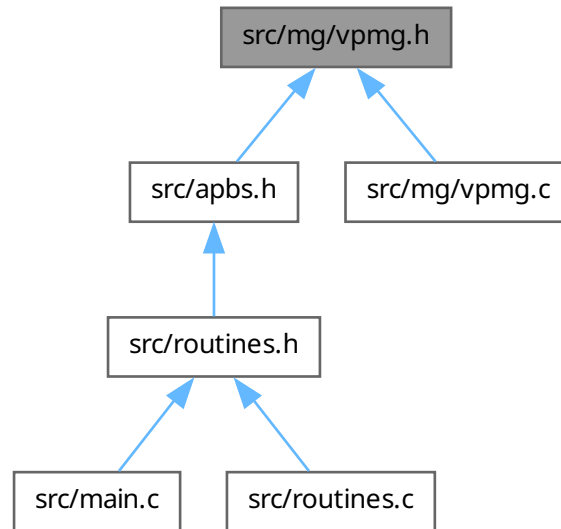
Contains declarations for class Vpmg.

```
#include "apbscfg.h"
#include "maloc/maloc.h"
#include "generic/vhal.h"
#include "generic/vacc.h"
#include "generic/vcap.h"
#include "generic/vpbe.h"
#include "generic/mgparm.h"
#include "generic/pbeparm.h"
#include "generic/vmatrix.h"
#include "pmgc/mgdrvd.h"
#include "pmgc/newdrvd.h"
#include "pmgc/mgsubd.h"
#include "pmgc/mikpckd.h"
#include "pmgc/matvecd.h"
#include "mg/vpmgp.h"
#include "mg/vgrid.h"
```

Include dependency graph for vpmg.h:



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [sVpmg](#)

Contains public data members for Vpmg class/module.

Macros

- #define [VPMGMAXPART](#) 2000
- #define [VCUB](#)(x) ((x)*(x)*(x))
- #define [VLOG](#)(x) (log(x))
- #define [IJK](#)(i, j, k) (((k)*(nx)*(ny))+((j)*(nx))+(i))
- #define [IJKx](#)(j, k, i) (((i)*(ny)*(nz))+((k)*(ny))+(j))
- #define [IJKy](#)(i, k, j) (((j)*(nx)*(nz))+((k)*(nx))+(i))
- #define [IJKz](#)(i, j, k) (((k)*(nx)*(ny))+((j)*(nx))+(i))
- #define [VFCHI](#)(iint, iflt) (1.5+((double)(iint)-(iflt)))

Typedefs

- typedef struct [sVpmg](#) [Vpmg](#)

Declaration of the Vpmg class as the Vpmg structure.

Functions

- VEXTERNC unsigned long int [Vpmg_memChk](#) ([Vpmg](#) *thee)
Return the memory used by this structure (and its contents) in bytes.
- VEXTERNC [Vpmg](#) * [Vpmg_ctor](#) ([Vpmgp](#) *parms, [Vpbe](#) *pbe, int focusFlag, [Vpmg](#) *pmgOLD, [MGparm](#) *mgparm, [PBEparm_calcEnergy](#) energyFlag)

Constructor for the Vpmg class (allocates new memory)

- VEXTERNC int [Vpmg_ctor2](#) (Vpmg *thee, Vpmgp *parms, Vpbe *pbe, int focusFlag, Vpmg *pmgOLD, MGparm *mgparm, PBEparm_calcEnergy energyFlag)

FORTRAN stub constructor for the Vpmg class (uses previously-allocated memory)

- VEXTERNC void [Vpmg_dtor](#) (Vpmg **thee)

Object destructor.

- VEXTERNC void [Vpmg_dtor2](#) (Vpmg *thee)

FORTRAN stub object destructor.

- VEXTERNC int [Vpmg_fillco](#) (Vpmg *thee, Vsurf_Meth surfMeth, double splineWin, Vchrg_Meth chargeMeth, int useDielXMap, Vgrid *dielXMap, int useDielYMap, Vgrid *dielYMap, int useDielZMap, Vgrid *dielZMap, int useKappaMap, Vgrid *kappaMap, int usePotMap, Vgrid *potMap, int useChargeMap, Vgrid *chargeMap)

Fill the coefficient arrays prior to solving the equation.

- VEXTERNC int [Vpmg_solve](#) (Vpmg *thee)

Solve the PBE using PMG.

- VEXTERNC int [Vpmg_solveLaplace](#) (Vpmg *thee)

Solve Poisson's equation with a homogeneous Laplacian operator using the solvent dielectric constant. This solution is performed by a sine wave decomposition.

- VEXTERNC double [Vpmg_energy](#) (Vpmg *thee, int extFlag)

Get the total electrostatic energy.

- VEXTERNC double [Vpmg_qfEnergy](#) (Vpmg *thee, int extFlag)

Get the "fixed charge" contribution to the electrostatic energy.

- VEXTERNC double [Vpmg_qfAtomEnergy](#) (Vpmg *thee, Vatom *atom)

Get the per-atom "fixed charge" contribution to the electrostatic energy.

- VEXTERNC double [Vpmg_qmEnergy](#) (Vpmg *thee, int extFlag)

Get the "mobile charge" contribution to the electrostatic energy.

- VEXTERNC double [Vpmg_dielEnergy](#) (Vpmg *thee, int extFlag)

Get the "polarization" contribution to the electrostatic energy.

- VEXTERNC double [Vpmg_dielGradNorm](#) (Vpmg *thee)

Get the integral of the gradient of the dielectric function.

- VEXTERNC int [Vpmg_force](#) (Vpmg *thee, double *force, int atomID, Vsurf_Meth srfr, Vchrg_Meth chgm)

Calculate the total force on the specified atom in units of $k_B T/AA$.

- VEXTERNC int [Vpmg_qfForce](#) (Vpmg *thee, double *force, int atomID, Vchrg_Meth chgm)

Calculate the "charge-field" force on the specified atom in units of $k_B T/AA$.

- VEXTERNC int [Vpmg_dbForce](#) (Vpmg *thee, double *dbForce, int atomID, Vsurf_Meth srfr)

Calculate the dielectric boundary forces on the specified atom in units of $k_B T/AA$.

- VEXTERNC int [Vpmg_ibForce](#) (Vpmg *thee, double *force, int atomID, Vsurf_Meth srfr)

Calculate the osmotic pressure on the specified atom in units of $k_B T/AA$.

- VEXTERNC void [Vpmg_setPart](#) (Vpmg *thee, double lowerCorner[3], double upperCorner[3], int bflags[6])

Set partition information which restricts the calculation of observables to a (rectangular) subset of the problem domain.

- VEXTERNC void [Vpmg_unsetPart](#) (Vpmg *thee)

Remove partition restrictions.

- VEXTERNC int [Vpmg_fillArray](#) (Vpmg *thee, double *vec, Vdata_Type type, double parm, Vhal_PBEType pbe-type, PBEparm *pbeparm)

Fill the specified array with accessibility values.

- VPUBLIC void [Vpmg_fieldSpline4](#) (Vpmg *thee, int atomID, double field[3])

Computes the field at an atomic center using a stencil based on the first derivative of a 5th order B-spline.

- VEXTERNC double [Vpmg_qfPermanentMultipoleEnergy](#) (Vpmg *thee, int atomID)

Computes the permanent multipole electrostatic hydration energy (the polarization component of the hydration energy currently computed in TINKER).

- VEXTERNC void [Vpmg_qfPermanentMultipoleForce](#) ([Vpmg](#) *thee, int atomID, double force[3], double torque[3])

Computes the q-Phi Force for permanent multipoles based on 5th order B-splines.

- VEXTERNC void [Vpmg_ibPermanentMultipoleForce](#) ([Vpmg](#) *thee, int atomID, double force[3])

Compute the ionic boundary force for permanent multipoles.

- VEXTERNC void [Vpmg_dbPermanentMultipoleForce](#) ([Vpmg](#) *thee, int atomID, double force[3])

Compute the dielectric boundary force for permanent multipoles.

- VEXTERNC void [Vpmg_qfDirectPolForce](#) ([Vpmg](#) *thee, [Vgrid](#) *perm, [Vgrid](#) *induced, int atomID, double force[3], double torque[3])

q-Phi direct polarization force between permanent multipoles and induced dipoles, which are induced by the sum of the permanent intramolecular field and the permanent reaction field.

- VEXTERNC void [Vpmg_qfNLDirectPolForce](#) ([Vpmg](#) *thee, [Vgrid](#) *perm, [Vgrid](#) *nlInduced, int atomID, double force[3], double torque[3])

q-Phi direct polarization force between permanent multipoles and non-local induced dipoles based on 5th Order B-Splines. Keep in mind that the "non-local" induced dipoles are just a mathematical quantity that result from differentiation of the AMOEBA polarization energy.

- VEXTERNC void [Vpmg_ibDirectPolForce](#) ([Vpmg](#) *thee, [Vgrid](#) *perm, [Vgrid](#) *induced, int atomID, double force[3])

Ionic boundary direct polarization force between permanent multipoles and induced dipoles, which are induced by the sum of the permanent intramolecular field and the permanent reaction field.

- VEXTERNC void [Vpmg_ibNLDirectPolForce](#) ([Vpmg](#) *thee, [Vgrid](#) *perm, [Vgrid](#) *nlInduced, int atomID, double force[3])

Ionic boundary direct polarization force between permanent multipoles and non-local induced dipoles based on 5th order. Keep in mind that the "non-local" induced dipoles are just a mathematical quantity that result from differentiation of the AMOEBA polarization energy.

- VEXTERNC void [Vpmg_dbDirectPolForce](#) ([Vpmg](#) *thee, [Vgrid](#) *perm, [Vgrid](#) *induced, int atomID, double force[3])

Dielectric boundary direct polarization force between permanent multipoles and induced dipoles, which are induced by the sum of the permanent intramolecular field and the permanent reaction field.

- VEXTERNC void [Vpmg_dbNLDirectPolForce](#) ([Vpmg](#) *thee, [Vgrid](#) *perm, [Vgrid](#) *nlInduced, int atomID, double force[3])

Dielectric boundary direct polarization force between permanent multipoles and non-local induced dipoles. Keep in mind that the "non-local" induced dipoles are just a mathematical quantity that result from differentiation of the AMOEBA polarization energy.

- VEXTERNC void [Vpmg_qfMutualPolForce](#) ([Vpmg](#) *thee, [Vgrid](#) *induced, [Vgrid](#) *nlInduced, int atomID, double force[3])

Mutual polarization force for induced dipoles based on 5th order B-Splines. This force arises due to self-consistent convergence of the solute induced dipoles and reaction field.

- VEXTERNC void [Vpmg_ibMutualPolForce](#) ([Vpmg](#) *thee, [Vgrid](#) *induced, [Vgrid](#) *nlInduced, int atomID, double force[3])

Ionic boundary mutual polarization force for induced dipoles based on 5th order B-Splines. This force arises due to self-consistent convergence of the solute induced dipoles and reaction field.

- VEXTERNC void [Vpmg_dbMutualPolForce](#) ([Vpmg](#) *thee, [Vgrid](#) *induced, [Vgrid](#) *nlInduced, int atomID, double force[3])

Dielectric boundary mutual polarization force for induced dipoles based on 5th order B-Splines. This force arises due to self-consistent convergence of the solute induced dipoles and reaction field.

- VEXTERNC void [Vpmg_printColComp](#) ([Vpmg](#) *thee, char path[72], char title[72], char mxtype[3], int flag)

Print out a column-compressed sparse matrix in Harwell-Boeing format.

- VPRIVATE void [bcolcomp](#) (int *iparm, double *rparm, int *iwork, double *rwork, double *values, int *rowind, int *colptr, int *flag)

Build a column-compressed matrix in Harwell-Boeing format.

- VPRIVATE void [bcolcomp2](#) (int *iparm, double *rparm, int *nx, int *ny, int *nz, int *iz, int *ipc, double *rpc, double *ac, double *cc, double *values, int *rowind, int *colptr, int *flag)
Build a column-compressed matrix in Harwell-Boeing format.
- VPRIVATE void [bcolcomp3](#) (int *nx, int *ny, int *nz, int *ipc, double *rpc, double *ac, double *cc, double *values, int *rowind, int *colptr, int *flag)
Build a column-compressed matrix in Harwell-Boeing format.
- VPRIVATE void [bcolcomp4](#) (int *nx, int *ny, int *nz, int *ipc, double *rpc, double *oC, double *cc, double *oE, double *oN, double *uC, double *values, int *rowind, int *colptr, int *flag)
Build a column-compressed matrix in Harwell-Boeing format.
- VPRIVATE void [pcolcomp](#) (int *nrow, int *ncol, int *nnzero, double *values, int *rowind, int *colptr, char *path, char *title, char *mxtype)
Print a column-compressed matrix in Harwell-Boeing format.
- VPRIVATE double [bspline2](#) (double x)
Evaluate a cubic B-spline.
- VPRIVATE double [dbspline2](#) (double x)
Evaluate a cubic B-spline derivative.
- VPRIVATE double [VFCHI4](#) (int i, double f)
Return 2.5 plus difference of i - f.
- VPRIVATE double [bspline4](#) (double x)
Evaluate a 5th Order B-Spline (4th order polynomial)
- VPRIVATE double [dbspline4](#) (double x)
Evaluate a 5th Order B-Spline derivative (4th order polynomial)
- VPRIVATE double [d2bspline4](#) (double x)
Evaluate the 2nd derivative of a 5th Order B-Spline.
- VPRIVATE double [d3bspline4](#) (double x)
Evaluate the 3rd derivative of a 5th Order B-Spline.
- VPRIVATE double [Vpmg_polarizEnergy](#) (Vpmg *thee, int extFlag)
Determines energy from polarizeable charge and interaction with fixed charges according to Rocchia et al.
- VPRIVATE double [Vpmg_qfEnergyPoint](#) (Vpmg *thee, int extFlag)
Calculates charge-potential energy using summation over delta function positions (i.e. something like an Linf norm)
- VPRIVATE double [Vpmg_qfEnergyVolume](#) (Vpmg *thee, int extFlag)
Calculates charge-potential energy as integral over a volume.
- VPRIVATE void [Vpmg_splineSelect](#) (int srfm, Vpmg *acc, double *gpos, double win, double infrad, Vatom *atom, double *force)
Selects a spline based surface method from either VSM_SPLINE, VSM_SPLINE5 or VSM_SPLINE7.
- VPRIVATE void [bcfl1](#) (double size, double *apos, double charge, double xkappa, double pre1, double *gxcf, double *gycf, double *gzcf, double *xf, double *yf, double *zf, int nx, int ny, int nz)
*Increment all boundary points by $pre1 * (charge/d) * (exp(-xkappa * (d-size)) / (1 + xkappa * size))$ to add the effect of the Debye-Huckel potential due to a single charge.*
- VPRIVATE void [multipolebc](#) (double r, double kappa, double eps_p, double eps_w, double rad, double tsr[3])
This routine serves bcfl2. It returns (in tsr) the contraction independent portion of the Debye-Huckel potential tensor for a spherical ion with a central charge, dipole and quadrupole. See the code for an in depth description.
- VPRIVATE void [bcCalc](#) (Vpmg *thee)
Fill boundary condition arrays.
- VPRIVATE void [fillCoef](#) (Vpmg *thee)
Top-level driver to fill all operator coefficient arrays.
- VPRIVATE void [fillCoefMap](#) (Vpmg *thee)
Fill operator coefficient arrays from pre-calculated maps.

- VPRIVATE void [fillCoefMol](#) ([Vpmg](#) *thee)
Fill operator coefficient arrays from a molecular surface calculation.
- VPRIVATE void [fillCoefMollon](#) ([Vpmg](#) *thee)
Fill ion (nonlinear) operator coefficient array from a molecular surface calculation.
- VPRIVATE void [fillCoefMolDiel](#) ([Vpmg](#) *thee)
Fill differential operator coefficient arrays from a molecular surface calculation.
- VPRIVATE void [fillCoefMolDielNoSmooth](#) ([Vpmg](#) *thee)
Fill differential operator coefficient arrays from a molecular surface calculation without smoothing.
- VPRIVATE void [fillCoefMolDielSmooth](#) ([Vpmg](#) *thee)
Fill differential operator coefficient arrays from a molecular surface calculation with smoothing.
- VPRIVATE void [fillCoefSpline](#) ([Vpmg](#) *thee)
Fill operator coefficient arrays from a spline-based surface calculation.
- VPRIVATE void [fillCoefSpline3](#) ([Vpmg](#) *thee)
Fill operator coefficient arrays from a 5th order polynomial based surface calculation.
- VPRIVATE void [fillCoefSpline4](#) ([Vpmg](#) *thee)
Fill operator coefficient arrays from a 7th order polynomial based surface calculation.
- VPRIVATE Vrc_Codes [fillCoCharge](#) ([Vpmg](#) *thee)
Top-level driver to fill source term charge array.
- VPRIVATE Vrc_Codes [fillCoChargeMap](#) ([Vpmg](#) *thee)
Fill source term charge array from a pre-calculated map.
- VPRIVATE void [fillCoChargeSpline1](#) ([Vpmg](#) *thee)
Fill source term charge array from linear interpolation.
- VPRIVATE void [fillCoChargeSpline2](#) ([Vpmg](#) *thee)
Fill source term charge array from cubic spline interpolation.
- VPRIVATE void [fillCoPermanentMultipole](#) ([Vpmg](#) *thee)
Fill source term charge array for the use of permanent multipoles.
- VPRIVATE void [fillCoInducedDipole](#) ([Vpmg](#) *thee)
Fill source term charge array for use of induced dipoles.
- VPRIVATE void [fillCoNLInducedDipole](#) ([Vpmg](#) *thee)
Fill source term charge array for non-local induced dipoles.
- VPRIVATE void [qfForceSpline1](#) ([Vpmg](#) *thee, double *force, int atomID)
Charge-field force due to a linear spline charge function.
- VPRIVATE void [qfForceSpline2](#) ([Vpmg](#) *thee, double *force, int atomID)
Charge-field force due to a cubic spline charge function.
- VPRIVATE void [qfForceSpline4](#) ([Vpmg](#) *thee, double *force, int atomID)
Charge-field force due to a quintic spline charge function.
- VPRIVATE void [zlapSolve](#) ([Vpmg](#) *thee, double **solution, double **source, double **work1)
Calculate the solution to Poisson's equation with a simple Laplacian operator and zero-valued Dirichlet boundary conditions. Store the solution in thee->u.
- VPRIVATE void [markSphere](#) (double rtot, double *tpos, int nx, int ny, int nz, double hx, double hy, double hzed, double xmin, double ymin, double zmin, double *array, double markVal)
Mark the grid points inside a sphere with a particular value. This marks by resetting the the grid points inside the sphere to the specified value.
- VPRIVATE double [Vpmg_qmEnergySMPBE](#) ([Vpmg](#) *thee, int extFlag)
Vpmg_qmEnergy for SMPBE.
- VPRIVATE double [Vpmg_qmEnergyNONLIN](#) ([Vpmg](#) *thee, int extFlag)

9.108.1 Detailed Description

Contains declarations for class Vpmg.

Version

\$Id\$

Author

Nathan A. Baker

Attention

```
*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
* Nathan A. Baker (nathan.baker@pnnl.gov)
* Pacific Northwest National Laboratory
*
* Additional contributing authors listed in the code documentation.
*
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*
*

```

Definition in file [vpmg.h](#).

9.108.2 Macro Definition Documentation

9.108.2.1 IJK

```

#define IJK(
    i,
    j,
    k ) ((k)*(nx)*(ny)) + ((j)*(nx)) + (i)

```

Definition at line [1395](#) of file [vpmg.h](#).

9.108.2.2 IJKx

```

#define IJKx(
    j,
    k,
    i ) ((i)*(ny)*(nz)) + ((k)*(ny)) + (j)

```

Definition at line [1396](#) of file [vpmg.h](#).

9.108.2.3 IJKy

```

#define IJKy(
    i,
    k,
    j ) ((j)*(nx)*(nz)) + ((k)*(nx)) + (i)

```

Definition at line [1397](#) of file [vpmg.h](#).

9.108.2.4 IJKz

```

#define IJKz(
    i,
    j,
    k ) ((k)*(nx)*(ny)) + ((j)*(nx)) + (i)

```

Definition at line [1398](#) of file [vpmg.h](#).

9.108.2.5 VCUB

```

#define VCUB(
    x ) ((x)*(x)*(x))

```

Definition at line [1392](#) of file [vpmg.h](#).

9.108.2.6 VFCHI

```

#define VFCHI(
    iint,
    iflt ) (1.5+((double)(iint)-(iflt)))

```

Definition at line [1399](#) of file [vpmg.h](#).

9.108.2.7 VLOG

```
#define VLOG(
    x ) (log(x))
```

Definition at line 1393 of file [vpmg.h](#).

9.108.2.8 VPMGMAXPART

```
#define VPMGMAXPART 2000
```

Definition at line 105 of file [vpmg.h](#).

9.108.3 Function Documentation

9.108.3.1 bcCalc()

```
VPRIVATE void bcCalc (
    Vpmg * thee )
```

Fill boundary condition arrays.

Author

Nathan Baker

Definition at line 4382 of file [vpmg.c](#).

9.108.3.2 bcf11()

```
VPRIVATE void bcf11 (
    double size,
    double * apos,
    double charge,
    double xkappa,
    double pre1,
    double * gxcf,
    double * gycf,
    double * gzcf,
    double * xf,
    double * yf,
    double * zf,
    int nx,
    int ny,
    int nz )
```

Increment all boundary points by $pre1 * (charge/d) * (exp(-xkappa * (d-size)) / (1 + xkappa * size))$ to add the effect of the Debye-Huckel potential due to a single charge.

Author

Nathan Baker

Parameters

<i>apos</i>	Size of the ion
<i>charge</i>	Position of the ion
<i>xkappa</i>	Charge of the ion
<i>pre1</i>	Exponential screening factor
<i>gxcf</i>	Unit- and dielectric-dependent prefactor

Parameters

<i>gycf</i>	Set to x-boundary values
<i>gzcf</i>	Set to y-boundary values
<i>xf</i>	Set to z-boundary values
<i>yf</i>	Boundary point x-coordinates
<i>zf</i>	Boundary point y-coordinates
<i>nx</i>	Boundary point z-coordinates
<i>ny</i>	Number of grid points in x-direction
<i>nz</i>	Number of grid points in y-direction Number of grid points in y-direction

Definition at line [2564](#) of file [vpmg.c](#).

9.108.3.3 bspline2()

```
VPRIVATE double bspline2 (
    double x )
```

Evaluate a cubic B-spline.

Author

Nathan Baker

Returns

Cubic B-spline value

Parameters

<i>x</i>	Position
----------	----------

Definition at line [5496](#) of file [vpmg.c](#).

9.108.3.4 bspline4()

```
VPRIVATE double bspline4 (
    double x )
```

Evaluate a 5th Order B-Spline (4th order polynomial)

Author

: Michael Schnieders

Returns

5th Order B-Spline

Parameters

<i>x</i>	Position
----------	----------

Definition at line [7136](#) of file [vpmg.c](#).

9.108.3.5 d2bspline4()

```
VPRIVATE double d2bspline4 (  
    double x )
```

Evaluate the 2nd derivative of a 5th Order B-Spline.

Author

: Michael Schnieders

Returns

2nd derivative of a 5th Order B-Spline

Parameters

x	Position
---	----------

Definition at line [7202](#) of file [vpmg.c](#).

9.108.3.6 d3bspline4()

```
VPRIVATE double d3bspline4 (  
    double x )
```

Evaluate the 3rd derivative of a 5th Order B-Spline.

Author

: Michael Schnieders

Returns

3rd derivative of a 5th Order B-Spline

Parameters

x	Position
---	----------

Definition at line [7229](#) of file [vpmg.c](#).

9.108.3.7 dbspline2()

```
VPRIVATE double dbspline2 (  
    double x )
```

Evaluate a cubic B-spline derivative.

Author

Nathan Baker

Returns

Cubic B-spline derivative

Parameters

<i>x</i>	Position
----------	----------

Definition at line 5512 of file [vpmg.c](#).

9.108.3.8 db spline4()

```
VPRIVATE double db spline4 (  
    double x )
```

Evaluate a 5th Order B-Spline derivative (4th order polynomial)

Author

: Michael Schnieders

Returns

5th Order B-Spline derivative

Parameters

<i>x</i>	Position
----------	----------

Definition at line 7170 of file [vpmg.c](#).

9.108.3.9 fillcoCharge()

```
VPRIVATE Vrc_Codes fillcoCharge (  
    Vpmg * thee )
```

Top-level driver to fill source term charge array.

Returns

Success/failure status

Author

Nathan Baker

Definition at line 5287 of file [vpmg.c](#).

9.108.3.10 fillcoChargeMap()

```
VPRIVATE Vrc_Codes fillcoChargeMap (  
    Vpmg * thee )
```

Fill source term charge array from a pre-calculated map.

Returns

Success/failure status

Author

Nathan Baker

Definition at line 5343 of file [vpmg.c](#).

9.108.3.11 fillcoChargeSpline1()

```
VPRIVATE void fillcoChargeSpline1 (  
    Vpmg * thee )
```

Fill source term charge array from linear interpolation.

Author

Nathan Baker

Definition at line 5391 of file [vpmg.c](#).

9.108.3.12 fillcoChargeSpline2()

```
VPRIVATE void fillcoChargeSpline2 (  
    Vpmg * thee )
```

Fill source term charge array from cubic spline interpolation.

Author

Nathan Baker

Definition at line 5528 of file [vpmg.c](#).

9.108.3.13 fillcoCoef()

```
VPRIVATE void fillcoCoef (  
    Vpmg * thee )
```

Top-level driver to fill all operator coefficient arrays.

Author

Nathan Baker

Definition at line 5247 of file [vpmg.c](#).

9.108.3.14 fillcoCoefMap()

```
VPRIVATE void fillcoCoefMap (  
    Vpmg * thee )
```

Fill operator coefficient arrays from pre-calculated maps.

Author

Nathan Baker

Definition at line 4489 of file [vpmg.c](#).

9.108.3.15 fillcoCoefMol()

```
VPRIVATE void fillcoCoefMol (  
    Vpmg * thee )
```

Fill operator coefficient arrays from a molecular surface calculation.

Author

Nathan Baker

Definition at line 4612 of file [vpmg.c](#).

9.108.3.16 fillcoCoefMolDiel()

```
VPRIVATE void fillcoCoefMolDiel (  
    Vpmg * thee )
```

Fill differential operator coefficient arrays from a molecular surface calculation.

Author

Nathan Baker

Definition at line 4726 of file [vpmg.c](#).

9.108.3.17 fillcoCoefMolDielNoSmooth()

```
VPRIVATE void fillcoCoefMolDielNoSmooth (  
    Vpmg * thee )
```

Fill differential operator coefficient arrays from a molecular surface calculation without smoothing.

Author

Nathan Baker

Definition at line 4737 of file [vpmg.c](#).

9.108.3.18 fillcoCoefMolDielSmooth()

```
VPRIVATE void fillcoCoefMolDielSmooth (  
    Vpmg * thee )
```

Fill differential operator coefficient arrays from a molecular surface calculation with smoothing.

Molecular surface, dielectric smoothing following an implementation of Bruccoleri, et al. J Comput Chem 18 268-276 (1997).

This algorithm uses a 9 point harmonic smoothing technique - the point in question and all grid points 1/sqrt(2) grid spacings away.

Note

This uses thee->a1cf, thee->a2cf, thee->a3cf as temporary storage.

Author

Todd Dolinsky

Definition at line 4891 of file [vpmg.c](#).

9.108.3.19 fillcoCoefMolIon()

```
VPRIVATE void fillcoCoefMolIon (  
    Vpmg * thee )
```

Fill ion (nonlinear) operator coefficient array from a molecular surface calculation.

Author

Nathan Baker

Definition at line 4628 of file [vpmg.c](#).

9.108.3.20 fillcoCoefSpline()

```
VPRIVATE void fillcoCoefSpline (  
    Vpmg * thee )
```

Fill operator coefficient arrays from a spline-based surface calculation.

Author

Nathan Baker

Definition at line [5022](#) of file [vpmg.c](#).

9.108.3.21 fillcoCoefSpline3()

```
VPRIVATE void fillcoCoefSpline3 (  
    Vpmg * thee )
```

Fill operator coefficient arrays from a 5th order polynomial based surface calculation.

Author

Michael Schnieders

Definition at line [10430](#) of file [vpmg.c](#).

9.108.3.22 fillcoCoefSpline4()

```
VPRIVATE void fillcoCoefSpline4 (  
    Vpmg * thee )
```

Fill operator coefficient arrays from a 7th order polynomial based surface calculation.

Author

Michael Schnieders

Definition at line [9939](#) of file [vpmg.c](#).

9.108.3.23 fillcoInducedDipole()

```
VPRIVATE void fillcoInducedDipole (  
    Vpmg * thee )
```

Fill source term charge array for use of induced dipoles.

Author

Michael Schnieders

9.108.3.24 fillcoNLInducedDipole()

```
VPRIVATE void fillcoNLInducedDipole (  
    Vpmg * thee )
```

Fill source term charge array for non-local induced dipoles.

Author

Michael Schnieders

9.108.3.25 fillcoPermanentMultipole()

```
VPRIVATE void fillcoPermanentMultipole (
    Vpmg * thee )
```

Fill source term charge array for the use of permanent multipoles.

Author

Michael Schnieders

Definition at line 7240 of file [vpmg.c](#).

9.108.3.26 markSphere()

```
VPRIVATE void markSphere (
    double rtot,
    double * tpos,
    int nx,
    int ny,
    int nz,
    double hx,
    double hy,
    double hz,
    double xmin,
    double ymin,
    double zmin,
    double * array,
    double markVal )
```

Mark the grid points inside a sphere with a particular value. This marks by resetting the the grid points inside the sphere to the specified value.

Author

Nathan Baker

Parameters

<i>tpos</i>	Sphere radius
<i>nx</i>	Sphere position
<i>ny</i>	Number of grid points
<i>nz</i>	Number of grid points
<i>hx</i>	Number of grid points
<i>hy</i>	Grid spacing
<i>hz</i>	Grid spacing
<i>xmin</i>	Grid spacing
<i>ymin</i>	Grid lower corner
<i>zmin</i>	Grid lower corner
<i>array</i>	Grid lower corner
<i>markVal</i>	Grid values Value to mark with

Definition at line 6849 of file [vpmg.c](#).

9.108.3.27 multipolebc()

```
VPRIVATE void multipolebc (  
    double r,  
    double kappa,  
    double eps_p,  
    double eps_w,  
    double rad,  
    double tsr[3] )
```

This routine serves bcf12. It returns (in tsr) the contraction independent portion of the Debye-Huckel potential tensor for a spherical ion with a central charge, dipole and quadrupole. See the code for an in depth description.

Author

Michael Schnieders

Parameters

<i>kappa</i>	Distance to the boundary
<i>eps</i> _{↔ _p}	Exponential screening factor
<i>eps</i> _{↔ _w}	Solute dielectric
<i>rad</i>	Solvent dielectric
<i>tsr</i>	Radius of the sphere Contraction-independent portion of each tensor

Definition at line 3487 of file [vpmg.c](#).

9.108.3.28 qfForceSpline1()

```
VPRIVATE void qfForceSpline1 (  
    Vpmg * thee,  
    double * force,  
    int atomID )
```

Charge-field force due to a linear spline charge function.

Author

Nathan Baker

Parameters

<i>atomID</i>	Set to force Valist atom ID
---------------	-----------------------------

Definition at line 6311 of file [vpmg.c](#).

9.108.3.29 qfForceSpline2()

```
VPRIVATE void qfForceSpline2 (  
    Vpmg * thee,  
    double * force,  
    int atomID )
```

Charge-field force due to a cubic spline charge function.

Author

Nathan Baker

Parameters

<i>atomID</i>	Set to force Valist atom ID
---------------	-----------------------------

Definition at line 6448 of file [vpmg.c](#).**9.108.3.30 qfForceSpline4()**

```
VPRIVATE void qfForceSpline4 (  
    Vpmg * thee,  
    double * force,  
    int atomID )
```

Charge-field force due to a quintic spline charge function.

Author

Michael Schnieders

Parameters

<i>atomID</i>	Set to force Valist atom ID
---------------	-----------------------------

Definition at line 6561 of file [vpmg.c](#).**9.108.3.31 VFCHI4()**

```
VPRIVATE double VFCHI4 (  
    int i,  
    double f )
```

Return 2.5 plus difference of i - f.

Author

Michael Schnieders

Returns

(2.5+((double)(i)-(f)))

Definition at line 7132 of file [vpmg.c](#).**9.108.3.32 Vpmg_polarizEnergy()**

```
VPRIVATE double Vpmg_polarizEnergy (  
    Vpmg * thee,  
    int extFlag )
```

Determines energy from polarizeable charge and interaction with fixed charges according to Rocchia et al.

Author

Nathan Baker

Returns

Energy in kT

Parameters

<i>extFlag</i>	If 1, add external energy contributions to result
----------------	---

Definition at line 1148 of file [vpmg.c](#).

9.108.3.33 Vpmg_qfEnergyPoint()

```
VPRIVATE double Vpmg_qfEnergyPoint (
    Vpmg * thee,
    int extFlag )
```

Calculates charge-potential energy using summation over delta function positions (i.e. something like an Linf norm)

Author

Nathan Baker

Returns

Energy in kT

Parameters

<i>extFlag</i>	If 1, add external energy contributions to result
----------------	---

Definition at line 1704 of file [vpmg.c](#).

9.108.3.34 Vpmg_qfEnergyVolume()

```
VPRIVATE double Vpmg_qfEnergyVolume (
    Vpmg * thee,
    int extFlag )
```

Calculates charge-potential energy as integral over a volume.

Author

Nathan Baker

Returns

Energy in kT

Parameters

<i>extFlag</i>	If 1, add external energy contributions to result
----------------	---

Definition at line 1861 of file [vpmg.c](#).

9.108.3.35 Vpmg_qmEnergyNONLIN()

```
VPRIVATE double Vpmg_qmEnergyNONLIN (
    Vpmg * thee,
    int extFlag )
```

Definition at line 1401 of file [vpmg.c](#).

9.108.3.36 Vpmg_qmEnergySMPBE()

```
VPRIVATE double Vpmg_qmEnergySMPBE (
    Vpmg * thee,
    int extFlag )
```

Vpmg_qmEnergy for SMPBE.

Author

Vincent Chu

Definition at line 1490 of file [vpmg.c](#).

9.108.3.37 Vpmg_splineSelect()

```
VPRIVATE void Vpmg_splineSelect (
    int srfm,
    Vacc * acc,
    double * gpos,
    double win,
    double infrad,
    Vatom * atom,
    double * force )
```

Selects a spline based surface method from either VSM_SPLINE, VSM_SPLINE5 or VSM_SPLINE7.

Author

David Gohara

Parameters

<i>acc</i>	Surface method, currently VSM_SPLINE, VSM_SPLINE5, or VSM_SPLINE7
<i>gpos</i>	Accessibility object
<i>win</i>	Position array -> array[3]
<i>infrad</i>	Spline window
<i>atom</i>	Inflation radius
<i>force</i>	Atom object Force array -> array[3]

Definition at line 1893 of file [vpmg.c](#).

9.108.3.38 zlapSolve()

```
VPRIVATE void zlapSolve (
    Vpmg * thee,
    double ** solution,
    double ** source,
    double ** work1 )
```

Calculate the solution to Poisson's equation with a simple Laplacian operator and zero-valued Dirichlet boundary condi-

tions. Store the solution in thee->u.

Author

Nathan Baker

Note

Vpmg_fillco must be called first

Parameters

<i>source</i>	Solution term vector
<i>work1</i>	Source term vector Work vector

Definition at line 6898 of file vpmg.c.

9.109 vpmg.h

[Go to the documentation of this file.](#)

```

00001
00080 #ifndef _VPMG_H_
00081 #define _VPMG_H_
00082
00083 #include "apbscfg.h"
00084
00085 #include "malloc/malloc.h"
00086
00087 #include "generic/vhal.h"
00088 #include "generic/vacc.h"
00089 #include "generic/vcap.h"
00090 #include "generic/vpbe.h"
00091 #include "generic/mgparm.h"
00092 #include "generic/pbeparm.h"
00093 #include "generic/vmatrix.h"
00094 #include "pmgc/mgdrv.h"
00095 #include "pmgc/newdrv.h"
00096 #include "pmgc/mgsbd.h"
00097 #include "pmgc/mikpckd.h"
00098 #include "pmgc/matvecd.h"
00099 #include "mg/vpmgp.h"
00100 #include "mg/vgrid.h"
00101
00105 #define VPMGMAXPART 2000
00106
00116 struct sVpmg {
00117
00118     Vmem *vmem;
00119     Vpmgp *pmgp;
00120     Vpbe *pbe;
00122 #ifdef BURY_FORTRAN
00123     Vpde *pde;
00124     Vmgdriver *mgdriver;
00125 #endif
00126
00127     double *epsx;
00128     double *epsy;
00129     double *epsz;
00130     double *kappa;
00131     double *pot;
00132     double *charge;
00133     int *iparm;
00134     double *rparm;
00135     int *iwork;
00136     double *rwork;
00137     double *alcf;
00138     double *a2cf;
00142     double *a3cf;
00144     double *ccf;
00145     double *fcf;

```

```

00146 double *tcf;
00147 double *u;
00148 double *xf;
00149 double *yf;
00150 double *zf;
00151 double *gxcf;
00152 double *gycf;
00153 double *gzcf;
00154 double *pvec;
00155 double extDiEnergy;
00157 double extQmEnergy;
00159 double extQfEnergy;
00161 double extNpEnergy;
00163 Vsurf_Meth surfMeth;
00164 double splineWin;
00165 Vchrg_Meth chargeMeth;
00166 Vchrg_Src chargeSrc;
00168 int filled;
00170 int useDielXMap;
00172 Vgrid *dielXMap;
00173 int useDielYMap;
00175 Vgrid *dielYMap;
00176 int useDielZMap;
00178 Vgrid *dielZMap;
00179 int useKappaMap;
00181 Vgrid *kappaMap;
00182 int usePotMap;
00184 Vgrid *potMap;
00186 int useChargeMap;
00188 Vgrid *chargeMap;
00189 };
00190
00195 typedef struct sVpmg Vpmg;
00196
00197 /* ////////////////////////////////////////////////////////////////////
00200 #if !defined(VINLINE_VPMG)
00201
00208     VEXTERNC unsigned long int Vpmg_memChk(
00209         Vpmg *thee /**< Object for memory check */
00210     );
00211
00212 #else /* if defined(VINLINE_VPMG) */
00213 #   define Vpmg_memChk(thee) (Vmem_bytes((thee)->vmem))
00215
00216 #endif /* if !defined(VINLINE_VPMG) */
00217
00218 /* ////////////////////////////////////////////////////////////////////
00221
00226 VEXTERNC Vpmg* Vpmg_ctor(
00227     Vpmgp *parms, /**< PMG parameter object */
00228     Vpbe *pbe,
00229     int focusFlag,
00230     Vpmg *pmgOLD,
00231     MGparm *mgparm,
00232     PBEparm_calcEnergy energyFlag
00233 );
00234
00242 VEXTERNC int Vpmg_ctor2(
00243     Vpmg *thee,
00244     Vpmgp *parms,
00245     Vpbe *pbe,
00246     int focusFlag,
00247     Vpmg *pmgOLD,
00248     MGparm *mgparm,
00249     PBEparm_calcEnergy energyFlag
00251 );
00254
00255
00260 VEXTERNC void Vpmg_dtor(
00261     Vpmg **thee
00263 );
00264
00269 VEXTERNC void Vpmg_dtor2(
00270     Vpmg *thee
00271 );
00272
00281 VEXTERNC int Vpmg_fillco(
00282     Vpmg *thee,
00283     Vsurf_Meth surfMeth,
00284     double splineWin,
00286     Vchrg_Meth chargeMeth,

```

```
00287         int useDielXMap,
00288         Vgrid *dielXMap,
00289         int useDielYMap,
00290         Vgrid *dielYMap,
00291         int useDielZMap,
00292         Vgrid *dielZMap,
00293         int useKappaMap,
00294         Vgrid *kappaMap,
00295         int usePotMap,
00296         Vgrid *potMap,
00297         int useChargeMap,
00298         Vgrid *chargeMap
00299     );
00300
00306 VEXTERNC int Vpmg_solve(
00307     Vpmg *thee
00308 );
00309
00321 VEXTERNC int Vpmg_solveLaplace(
00322     Vpmg *thee
00323 );
00324
00334 VEXTERNC double Vpmg_energy(
00335     Vpmg *thee,
00336     int extFlag
00340 );
00341
00359 VEXTERNC double Vpmg_qfEnergy(
00360     Vpmg *thee,
00361     int extFlag
00365 );
00366
00386 VEXTERNC double Vpmg_qfAtomEnergy(
00387     Vpmg *thee,
00388     Vatom *atom
00389 );
00390
00415 VEXTERNC double Vpmg_qmEnergy(
00416     Vpmg *thee,
00417     int extFlag
00421 );
00422
00423
00442 VEXTERNC double Vpmg_dielEnergy(
00443     Vpmg *thee,
00444     int extFlag
00448 );
00449
00450
00467 VEXTERNC double Vpmg_dielGradNorm(
00468     Vpmg *thee
00469 );
00470
00482 VEXTERNC int Vpmg_force(
00483     Vpmg *thee,
00484     double *force,
00486     int atomID,
00487     Vsurf_Meth srfm,
00488     Vchrg_Meth chgm
00489 );
00490
00502 VEXTERNC int Vpmg_qfForce(
00503     Vpmg *thee,
00504     double *force,
00506     int atomID,
00507     Vchrg_Meth chgm
00508 );
00509
00521 VEXTERNC int Vpmg_dbForce(
00522     Vpmg *thee,
00523     double *dbForce,
00525     int atomID,
00526     Vsurf_Meth srfm
00527 );
00528
00540 VEXTERNC int Vpmg_ibForce(
00541     Vpmg *thee,
00542     double *force,
00544     int atomID,
00545     Vsurf_Meth srfm
00546 );
```

```

00547
00553 VEXTERNC void Vpmg_setPart (
00554     Vpmg *thee,
00555     double lowerCorner[3],
00556     double upperCorner[3],
00557     int bflags[6]
00561 );
00562
00567 VEXTERNC void Vpmg_unsetPart (
00568     Vpmg *thee
00569 );
00570
00576 VEXTERNC int Vpmg_fillArray (
00577     Vpmg *thee,
00578     double *vec,
00580     Vdata_Type type,
00581     double parm,
00582     Vhal_PBEType pbetype,
00583     PBEparm * pbeparm
00584 );
00585
00591 VPUBLIC void Vpmg_fieldSpline4 (
00592     Vpmg *thee,
00593     int atomID,
00594     double field[3]
00595 );
00596
00604 VEXTERNC double Vpmg_qfPermanentMultipoleEnergy (
00605     Vpmg *thee,
00606     int atomID
00607 );
00608
00614 VEXTERNC void Vpmg_qfPermanentMultipoleForce (
00615     Vpmg *thee,
00616     int atomID,
00617     double force[3],
00618     double torque[3]
00619 );
00620
00625 VEXTERNC void Vpmg_ibPermanentMultipoleForce (
00626     Vpmg *thee,
00627     int atomID,
00628     double force[3]
00629 );
00630
00635 VEXTERNC void Vpmg_dbPermanentMultipoleForce (
00636     Vpmg *thee,
00637     int atomID,
00638     double force[3]
00639 );
00640
00647 VEXTERNC void Vpmg_qfDirectPolForce (
00648     Vpmg *thee,
00649     Vgrid *perm,
00650     Vgrid *induced,
00651     int atomID,
00652     double force[3],
00653     double torque[3]
00654 );
00655
00664 VEXTERNC void Vpmg_qfNLDirectPolForce (
00665     Vpmg *thee,
00666     Vgrid *perm,
00667     Vgrid *nlInduced,
00668     int atomID,
00669     double force[3],
00670     double torque[3]
00671 );
00672
00680 VEXTERNC void Vpmg_ibDirectPolForce (
00681     Vpmg *thee,
00682     Vgrid *perm,
00683     Vgrid *induced,
00684     int atomID,
00685     double force[3]
00686 );
00687
00696 VEXTERNC void Vpmg_ibNLDirectPolForce (
00697     Vpmg *thee,
00698     Vgrid *perm,
00699     Vgrid *nlInduced,

```

```
00700         int atomID,
00701         double force[3]
00702     );
00703
00711 VEXTERNC void Vpmg_dbDirectPolForce(
00712     Vpmg *thee,
00713     Vgrid *perm,
00714     Vgrid *induced,
00715     int atomID,
00716     double force[3]
00717 );
00718
00727 VEXTERNC void Vpmg_dbNLDirectPolForce(
00728     Vpmg *thee,
00729     Vgrid *perm,
00730     Vgrid *nlInduced,
00731     int atomID,
00732     double force[3]
00733 );
00734
00741 VEXTERNC void Vpmg_qfMutualPolForce(
00742     Vpmg *thee,
00743     Vgrid *induced,
00744     Vgrid *nlInduced,
00745     int atomID,
00746     double force[3]
00747 );
00748
00756 VEXTERNC void Vpmg_ibMutualPolForce(
00757     Vpmg *thee,
00758     Vgrid *induced,
00759     Vgrid *nlInduced,
00760     int atomID,
00761     double force[3]
00762 );
00763
00771 VEXTERNC void Vpmg_dbMutualPolForce(
00772     Vpmg *thee,
00773     Vgrid *induced,
00774     Vgrid *nlInduced,
00775     int atomID,
00776     double force[3]
00777 );
00778
00785 VEXTERNC void Vpmg_printColComp(
00786     Vpmg *thee,
00787     char path[72],
00788     char title[72],
00789     char mxtype[3],
00790     int flag
00801 );
00802
00803
00804
00811 VPRIVATE void bcolcomp(
00812     int *iparm,
00813     double *rparm,
00814     int *iwork,
00815     double *rwork,
00816     double *values,
00817     int *rowind,
00818     int *colptr,
00819     int *flag
00824 );
00825
00826
00827
00834 VPRIVATE void bcolcomp2(
00835     int *iparm,
00836     double *rparm,
00837     int *nx,
00838     int *ny,
00839     int *nz,
00840     int *iz,
00841     int *ipc,
00842     double *rpc,
00843     double *ac,
00844     double *cc,
00845     double *values,
00846     int *rowind,
00847     int *colptr,
```

```

00848         int      *flag
00853     );
00854
00855
00856
00863 VPRIVATE void bcolcomp3(
00864     int      *nx,
00865     int      *ny,
00866     int      *nz,
00867     int      *ipc,
00868     double   *rpc,
00869     double   *ac,
00870     double   *cc,
00871     double   *values,
00872     int      *rowind,
00873     int      *colptr,
00874     int      *flag
00875 );
00876
00877
00878
00885 VPRIVATE void bcolcomp4(
00886     int      *nx,
00887     int      *ny,
00888     int      *nz,
00889     int      *ipc,
00890     double   *rpc,
00891     double   *oC,
00892     double   *cc,
00893     double   *oE,
00894     double   *oN,
00895     double   *uC,
00896     double   *values,
00897     int      *rowind,
00898     int      *colptr,
00899     int      *flag
00900 );
00901
00902
00903
00910 VPRIVATE void pcolcomp(
00911     int      *nrow,
00912     int      *ncol,
00913     int      *nnzero,
00914     double   *values,
00915     int      *rowind,
00916     int      *colptr,
00917     char     *path,
00918     char     *title,
00919     char     *mxtype
00920 );
00921
00922
00923
00924 /* ////////////////////////////////////////
00925 // Internal routines
00926
00927
00933 VPRIVATE double bspline2(
00934     double x /** Position */
00935 );
00936
00942 VPRIVATE double dbspline2(
00943     double x
00944 );
00945
00951 VPRIVATE double VFCHI4(
00952     int i,
00953     double f
00954 );
00955
00961 VPRIVATE double bspline4(
00962     double x
00963 );
00964
00970 VPRIVATE double dbspline4(
00971     double x
00972 );
00973
00979 VPRIVATE double d2bspline4(
00980     double x
00981 );

```



```
00982
00988 VPRIVATE double d3bspline4(
00989     double x
00990 );
00991
00998 VPRIVATE double Vpmg_polarizEnergy(
00999     Vpmg *thee,
01000     int extFlag
01002 );
01009 VPRIVATE double Vpmg_qfEnergyPoint(
01010     Vpmg *thee,
01011     int extFlag
01013 );
01014
01020 VPRIVATE double Vpmg_qfEnergyVolume(
01021     Vpmg *thee,
01022     int extFlag
01024 );
01025
01031 VPRIVATE void Vpmg_splineSelect(
01032     int srfm,
01034     Vacc *acc,
01035     double *gpos,
01036     double win,
01037     double infrad,
01038     Vatom *atom,
01039     double *force
01040 );
01041
01047 VPRIVATE void focusFillBound(
01048     Vpmg *thee,
01049     Vpmg *pmg
01050 );
01051
01058 VPRIVATE void bcfl1(
01059     double size,
01060     double *apos,
01061     double charge,
01062     double xkappa,
01063     double prel,
01064     double *gxcf,
01065     double *gycf,
01066     double *gzcf,
01067     double *xf,
01068     double *yf,
01069     double *zf,
01070     int nx,
01071     int ny,
01072     int nz
01073 );
01074
01080 VPRIVATE void bcfl2(
01081     double size,
01082     double *apos,
01083     double charge,
01084     double *dipole,
01085     double *quad,
01086     double xkappa,
01087     double eps_p,
01088     double eps_w,
01089     double T,
01090     double *gxcf,
01091     double *gycf,
01092     double *gzcf,
01093     double *xf,
01094     double *yf,
01095     double *zf,
01096     int nx,
01097     int ny,
01098     int nz
01099 );
01100
01109 VPRIVATE void multipolebc(
01110     double r,
01111     double kappa,
01112     double eps_p,
01113     double eps_w,
01114     double rad,
01115     double tsr[3]
01116 );
01117
```

```
01126 VPRIVATE double bcfillsp(  
01127     double size,  
01128     double *apos,  
01129     double charge,  
01130     double xkappa,  
01131     double prel,  
01132     double *pos  
01133 );  
01134  
01139 VPRIVATE void bcCalc(  
01140     Vpmg *thee  
01141 );  
01142  
01147 VPRIVATE void fillcoCoef(  
01148     Vpmg *thee  
01149 );  
01150  
01155 VPRIVATE void fillcoCoefMap(  
01156     Vpmg *thee  
01157 );  
01158  
01164 VPRIVATE void fillcoCoefMol(  
01165     Vpmg *thee  
01166 );  
01167  
01173 VPRIVATE void fillcoCoefMolIon(  
01174     Vpmg *thee  
01175 );  
01176  
01182 VPRIVATE void fillcoCoefMolDiel(  
01183     Vpmg *thee  
01184 );  
01185  
01191 VPRIVATE void fillcoCoefMolDielNoSmooth(  
01192     Vpmg *thee  
01193 );  
01194  
01208 VPRIVATE void fillcoCoefMolDielSmooth(  
01209     Vpmg *thee  
01210 );  
01211  
01217 VPRIVATE void fillcoCoefSpline(  
01218     Vpmg *thee  
01219 );  
01220  
01226 VPRIVATE void fillcoCoefSpline3(  
01227     Vpmg *thee  
01228 );  
01229  
01235 VPRIVATE void fillcoCoefSpline4(  
01236     Vpmg *thee  
01237 );  
01238  
01244 VPRIVATE Vrc_Codes fillcoCharge(  
01245     Vpmg *thee  
01246 );  
01247  
01253 VPRIVATE Vrc_Codes fillcoChargeMap(  
01254     Vpmg *thee  
01255 );  
01256  
01261 VPRIVATE void fillcoChargeSpline1(  
01262     Vpmg *thee  
01263 );  
01264  
01269 VPRIVATE void fillcoChargeSpline2(  
01270     Vpmg *thee  
01271 );  
01272  
01277 VPRIVATE void fillcoPermanentMultipole(  
01278     Vpmg *thee  
01279 );  
01280  
01285 VPRIVATE void fillcoInducedDipole(  
01286     Vpmg *thee  
01287 );  
01288  
01294 VPRIVATE void fillcoNLInducedDipole(  
01295     Vpmg *thee  
01296 );  
01297
```

```

01304 VPRIVATE void extEnergy(
01305     Vpmg *thee,
01306     Vpmg *pmgOLD,
01307     PBEparm_calcEnergy extFlag,
01308     double partMin[3],
01309     double partMax[3],
01310     int bflags[6]
01311 );
01312
01317 VPRIVATE void qfForceSpline1(
01318     Vpmg *thee,
01319     double *force,
01320     int atomID
01321 );
01322
01327 VPRIVATE void qfForceSpline2(
01328     Vpmg *thee,
01329     double *force,
01330     int atomID
01331 );
01332
01337 VPRIVATE void qfForceSpline4(
01338     Vpmg *thee,
01339     double *force,
01340     int atomID
01341 );
01342
01343
01351 VPRIVATE void zlapSolve(
01352     Vpmg *thee,
01353     double **solution,
01354     double **source,
01355     double **work1
01356 );
01357
01364 VPRIVATE void markSphere(
01365     double rtot,
01366     double *tpos,
01367     int nx,
01368     int ny,
01369     int nz,
01370     double hx,
01371     double hy,
01372     double hzed,
01373     double xmin,
01374     double ymin,
01375     double zmin,
01376     double *array,
01377     double markVal
01378 );
01379
01384 VPRIVATE double Vpmg_qmEnergySMPBE(Vpmg *thee, int extFlag);
01385 VPRIVATE double Vpmg_qmEnergyNONLIN(Vpmg *thee, int extFlag);
01386
01387
01388
01389 // Additional macros and definitions. May not be needed
01390
01391 // Added by Vincent Chu 9/13/06 for SMPB
01392 #define VCUB(x) ((x)*(x)*(x))
01393 #define VLOG(x) (log(x))
01394
01395 #define IJK(i,j,k) ((i)*(nx)*(ny))+((j)*(nx))+i)
01396 #define IJKx(j,k,i) ((i)*(ny)*(nz))+((k)*(ny))+j)
01397 #define IJKy(i,k,j) ((j)*(nx)*(nz))+((k)*(nx))+i)
01398 #define IJKz(i,j,k) ((i)*(nx)*(ny))+((j)*(nx))+i)
01399 #define VFCHI(iint,iflt) (1.5+((double)(iint)-(iflt)))
01400
01401
01402 #endif /* ifndef _VPMG_H_ */
01403

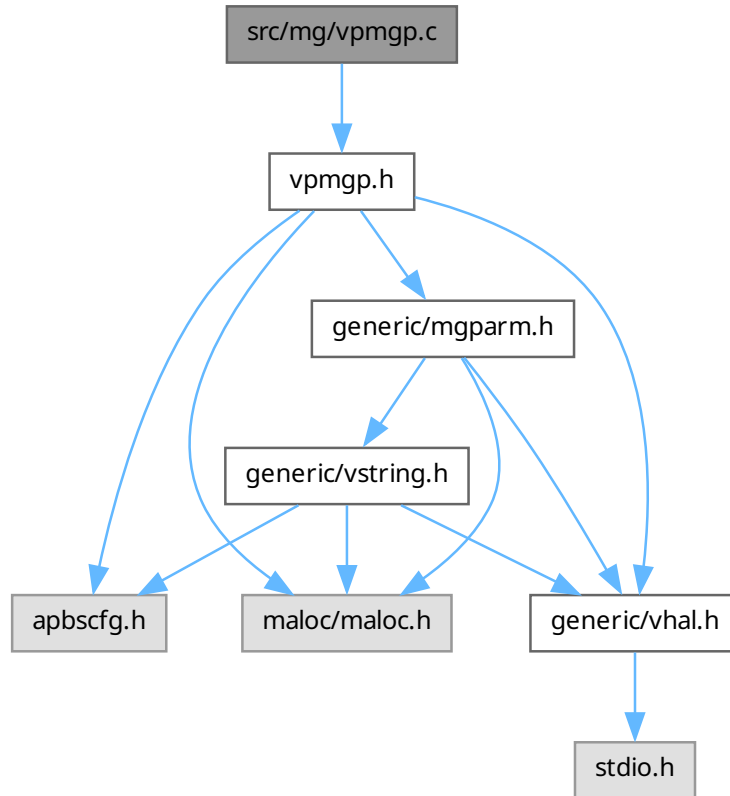
```

9.110 src/mg/vpmg.c File Reference

Class Vpmgp methods.

```
#include "vpmgp.h"
```

Include dependency graph for vpmgp.c:



Functions

- **VPUBLIC** [Vpmgp](#) * [Vpmgp_ctor](#) ([MGparm](#) *mgparm)
Construct PMG parameter object and initialize to default values.
- **VPUBLIC** int [Vpmgp_ctor2](#) ([Vpmgp](#) *thee, [MGparm](#) *mgparm)
FORTTRAN stub to construct PMG parameter object and initialize to default values.
- **VPUBLIC** void [Vpmgp_dtor](#) ([Vpmgp](#) **thee)
Object destructor.
- **VPUBLIC** void [Vpmgp_dtor2](#) ([Vpmgp](#) *thee)
FORTTRAN stub for object destructor.
- **VPUBLIC** void [Vpmgp_size](#) ([Vpmgp](#) *thee)
Determine array sizes and parameters for multigrid solver.
- **VPUBLIC** int [coarsenThis](#) (int nOld)
- **VPUBLIC** void [Vpmgp_makeCoarse](#) (int numLevel, int nxOld, int nyOld, int nzOld, int *nxNew, int *nyNew, int *nzNew)
Coarsen the grid by the desired number of levels and determine the resulting numbers of grid points.

9.110.1 Detailed Description

Class Vpmgp methods.

Author

Nathan Baker

Version

\$Id\$

Attention

```
*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
* Nathan A. Baker (nathan.baker@pnnl.gov)
* Pacific Northwest National Laboratory
*
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* THE POSSIBILITY OF SUCH DAMAGE.
*
*
```

Definition in file [vpmgp.c](#).

9.110.2 Function Documentation

9.110.2.1 coarsenThis()

```
VPRIVATE int coarsenThis (
```

```
int nOld )
```

Definition at line 294 of file [vpmgp.c](#).

9.111 vpmgp.c

[Go to the documentation of this file.](#)

```
00001
00057 #include "vpmgp.h"
00058
00059 VEMBED(rcsid="$Id$")
00060
00061 /* ////////////////////////////////////////////////////////////////////
00062 // Class Vpmgp: Inlineable methods
00064 #if !defined(VINLINE_VACC)
00065 #endif /* if !defined(VINLINE_VACC) */
00066
00067 /* ////////////////////////////////////////////////////////////////////
00068 // Class Vpmgp: Non-inlineable methods
00070
00071 /* ////////////////////////////////////////////////////////////////////
00072 // Routine: Vpmgp_ctor
00073 //
00074 // Author: Nathan Baker
00076 VPUBLIC Vpmgp* Vpmgp_ctor(MGparm *mgparm) {
00077
00078     Vpmgp *thee = VNULL;
00079
00080     /* Set up the structure */
00081     thee = (Vpmgp*)Vmem_malloc(VNULL, 1, sizeof(Vpmgp) );
00082     VASSERT( thee != VNULL);
00083     VASSERT(Vpmgp_ctor2(thee,mgparm));
00084
00085     return thee;
00086 }
00087
00088 /* ////////////////////////////////////////////////////////////////////
00089 // Routine: Vpmgp_ctor2
00090 //
00091 // Author: Nathan Baker
00093 VPUBLIC int Vpmgp_ctor2(Vpmgp *thee,MGparm *mgparm) {
00094
00095     /* Specified parameters */
00096     thee->nx = mgparm->dime[0];
00097     thee->ny = mgparm->dime[1];
00098     thee->nz = mgparm->dime[2];
00099     thee->hx = mgparm->grid[0];
00100     thee->hy = mgparm->grid[1];
00101     thee->hz = mgparm->grid[2];
00102     thee->xlen = ((double) (mgparm->dime[0]-1))*mgparm->grid[0];
00103     thee->ylen = ((double) (mgparm->dime[1]-1))*mgparm->grid[1];
00104     thee->zlen = ((double) (mgparm->dime[2]-1))*mgparm->grid[2];
00105     thee->nlev = mgparm->nlev;
00106
00107     thee->nonlin = mgparm->nonlotype;
00108     thee->meth = mgparm->method;
00109
00110 #ifdef DEBUG_MAC_OSX_OCL
00111 #include "mach_chud.h"
00112     if(kOpenCLAvailable)
00113         thee->meth = 4;
00114 #endif
00115
00116     if (thee->nonlin == NONLIN_LPBE) thee->ipkey = IPKEY_LPBE; /* LPBE case */
00117     else if(thee->nonlin == NONLIN_SMPBE) thee->ipkey = IPKEY_SMPBE; /* SMPBE case */
00118     else thee->ipkey = IPKEY_NPBE; /* NPBE standard case */
00119
00120     /* Default parameters */
00121     if (mgparm->setetol) { /* If etol is set by the user in APBS input file, then use this custom-defined
    etol */
00122         thee->errtol = mgparm->etol;
00123         Vnm_print(1, " Error tolerance (etol) is now set to user-defined \
00124 value: %g \n", thee->errtol);
00125         Vnm_print(0, "Error tolerance (etol) is now set to user-defined \
00126 value: %g \n", thee->errtol);
00127     } else thee->errtol = 1.0e-6; /* Here are a few comments. Mike had this set to
00128 * 1e-9; conventional wisdom sets this at 1e-6 for
00129 * the PBE; Ray Luo sets this at 1e-3 for his
```

```

00130      * accelerated PBE (for dynamics, etc.) */
00131      thee->itmax = 200;
00132      thee->istop = 1;
00133      thee->iinfo = 1;          /* I'd recommend either 1 (for debugging LPBE) or 2 (for debugging NPBE),
                                higher values give too much output */
00134
00135      thee->bcfl = BCFL_SDH;
00136      thee->key = 0;
00137      thee->iperf = 0;
00138      thee->mgcoar = 2;
00139      thee->mgkey = 0;
00140      thee->nul = 2;
00141      thee->nu2 = 2;
00142      thee->mgprol = 0;
00143      thee->mgdisc = 0;
00144      thee->omegal = 19.4e-1;
00145      thee->omegan = 9.0e-1;
00146      thee->ipcon = 3;
00147      thee->irite = 8;
00148      thee->xcent = 0.0;
00149      thee->ycent = 0.0;
00150      thee->zcent = 0.0;
00151
00152      /* Default value for all APBS runs */
00153      thee->mgsmoo = 1;
00154      if (thee->nonlin == NONLIN_NPBE || thee->nonlin == NONLIN_SMPBE) {
00155          /* SMPBE Added - SMPBE needs to mimic NPBE */
00156          Vnm_print(0, "Vpmp_ctor2: Using meth = 1, mgsolv = 0\n");
00157          thee->mgsolv = 0;
00158      } else {
00159          /* Most rigorous (good for testing) */
00160          Vnm_print(0, "Vpmp_ctor2: Using meth = 2, mgsolv = 1\n");
00161          thee->mgsolv = 1;
00162      }
00163
00164      /* TEMPORARY USEAQUA */
00165      /* If we are using aqua, our solution method is either VSOL_CMGGAqua or VSOL_NewtonAqua
00166      * so we need to temporarily override the mgsolve value and set it to 0
00167      */
00168      if(mgparm->useAqua == 1) thee->mgsolv = 0;
00169
00170      return 1;
00171 }
00172
00173 /* ////////////////////////////////////////
00174 // Routine: Vpmpg_dtor
00175 //
00176 // Author:  Nathan Baker
00177 VPUBLIC void Vpmpg_dtor(Vpmpg **thee) {
00178     if ((*thee) != VNULL) {
00179         Vpmpg_dtor2(*thee);
00180         Vmem_free(VNULL, 1, sizeof(Vpmpg), (void **)thee);
00181         (*thee) = VNULL;
00182     }
00183 }
00184
00185
00186 }
00187
00188 /* ////////////////////////////////////////
00189 // Routine: Vpmpg_dtor2
00190 //
00191 // Author:  Nathan Baker
00192 VPUBLIC void Vpmpg_dtor2(Vpmpg *thee) { ; }
00193
00194
00195
00196 VPUBLIC void Vpmpg_size(
00197     Vpmpg *thee
00198 )
00199 {
00200
00201     int num_nf = 0;
00202     int num_narr = 2;
00203     int num_narrc = 27;
00204     int nxf, nyf, nzf, level, num_nf_oper, num_narrc_oper, n_band, nc_band, num_band, iretot;
00205
00206     thee->nf = thee->nx * thee->ny * thee->nz;
00207     thee->narr = thee->nf;
00208     nxf = thee->nx;
00209     nyf = thee->ny;
00210     nzf = thee->nz;
00211     thee->nxc = thee->nx;

```

```

00212     thee->nyc = thee->ny;
00213     thee->nzc = thee->nz;
00214
00215     for (level=2; level<=thee->nlev; level++) {
00216         Vpmgp_makeCoarse(1, nxf, nyf, nzf, &(thee->nxc), &(thee->nyc), &(thee->nzc)); /* NAB TO-DO --
implement this function and check which variables need to be passed by reference... */
00217         nxf = thee->nxc;
00218         nyf = thee->nyc;
00219         nzf = thee->nzc;
00220         thee->narr = thee->narr + (nxf * nyf * nzf);
00221     }
00222
00223     thee->nc = thee->nxc * thee->nyc * thee->nzc;
00224     thee->narrc = thee->narr - thee->nf;
00225
00226     /* Box or FEM discretization on fine grid? */
00227     switch (thee->mgdisc) { /* NAB TO-DO: This needs to be changed into an enumeration */
00228     case 0:
00229         num_nf_oper = 4;
00230         break;
00231     case 1:
00232         num_nf_oper = 14;
00233         break;
00234     default:
00235         Vnm_print(2, "Vpmgp_size: Invalid mgdisc value (%d)!\n", thee->mgdisc);
00236         VASSERT(0);
00237     }
00238
00239     /* Galerkin or standard coarsening? */
00240     switch (thee->mgcoar) { /* NAB TO-DO: This needs to be changed into an enumeration */
00241     case 0:
00242         if (thee->mgdisc != 0) {
00243             Vnm_print(2, "Vpmgp_size: Invalid mgcoar value (%d); must be used with mgdisc 0!\n",
thee->mgcoar);
00244             VASSERT(0);
00245         }
00246         num_narrc_oper = 4;
00247         break;
00248     case 1:
00249         if (thee->mgdisc != 0) {
00250             Vnm_print(2, "Vpmgp_size: Invalid mgcoar value (%d); must be used with mgdisc 0!\n",
thee->mgcoar);
00251             VASSERT(0);
00252         }
00253         num_narrc_oper = 14;
00254         break;
00255     case 2:
00256         num_narrc_oper = 14;
00257         break;
00258     default:
00259         Vnm_print(2, "Vpmgp_size: Invalid mgcoar value (%d)!\n", thee->mgcoar);
00260         VASSERT(0);
00261     }
00262
00263     /* LINPACK storage on coarse grid */
00264     switch (thee->mgsolv) { /* NAB TO-DO: This needs to be changed into an enumeration */
00265     case 0:
00266         n_band = 0;
00267         break;
00268     case 1:
00269         if ( ( (thee->mgcoar == 0) || (thee->mgcoar == 1)) && (thee->mgdisc == 0) ) {
00270             num_band = 1 + (thee->nxc-2)*(thee->nyc-2);
00271         } else {
00272             num_band = 1 + (thee->nxc-2)*(thee->nyc-2) + (thee->nxc-2) + 1;
00273         }
00274         nc_band = (thee->nxc-2)*(thee->nyc-2)*(thee->nzc-2);
00275         n_band = nc_band * num_band;
00276         break;
00277     default:
00278         Vnm_print(2, "Vpmgp_size: Invalid mgsolv value (%d)!\n", thee->mgsolv);
00279         VASSERT(0);
00280     }
00281
00282     /* Real storage parameters */
00283     thee->n_rpc = 100*(thee->nlev+1);
00284
00285     /* Resulting total required for real storage */
00286     thee->n_rwk = num_narr*thee->narr + (size_t)(num_nf + num_nf_oper)*thee->nf + (size_t)(num_narrc +
num_narrc_oper)*thee->narrc + n_band + thee->n_rpc;
00287
00288     /* Integer storage parameters */

```



```

00289     thee->n_iz = 50*(thee->nlev+1);
00290     thee->n_ipc = 100*(thee->nlev+1);
00291     thee->niwk = thee->n_iz + thee->n_ipc;
00292 }
00293
00294 VPRIVATE int coarsenThis(int nOld) {
00295     int nOut;
00296
00297     nOut = (nOld - 1) / 2 + 1;
00298
00299     if (((nOut-1)*2) != (nOld-1)) {
00300         Vnm_print(2, "Vpmgp_makeCoarse: Warning! The grid dimensions you have chosen are not consistent
with the nlev you have specified!\n");
00301         Vnm_print(2, "Vpmgp_makeCoarse: This calculation will only work if you are running with mg-dummy
type.\n");
00302     }
00303     if (nOut < 1) {
00304         Vnm_print(2, "D'oh! You coarsened the grid below zero! How did you do that?\n");
00305         VASSERT(0);
00306     }
00307
00308     return nOut;
00309 }
00310
00311
00312 VPUBLIC void Vpmgp_makeCoarse(
00313     int numLevel,
00314     int nxOld,
00315     int nyOld,
00316     int nzOld,
00317     int *nxNew,
00318     int *nyNew,
00319     int *nzNew
00320 )
00321 {
00322     int nxtmp, nytmp, nztmp, iLevel;
00323
00324     for (iLevel=0; iLevel<numLevel; iLevel++) {
00325         nxtmp = *nxNew;
00326         nytmp = *nyNew;
00327         nztmp = *nzNew;
00328         *nxNew = coarsenThis(nxtmp);
00329         *nyNew = coarsenThis(nytmp);
00330         *nzNew = coarsenThis(nztmp);
00331     }
00332
00333 }
00334 }

```

9.112 src/mg/vpmg.h File Reference

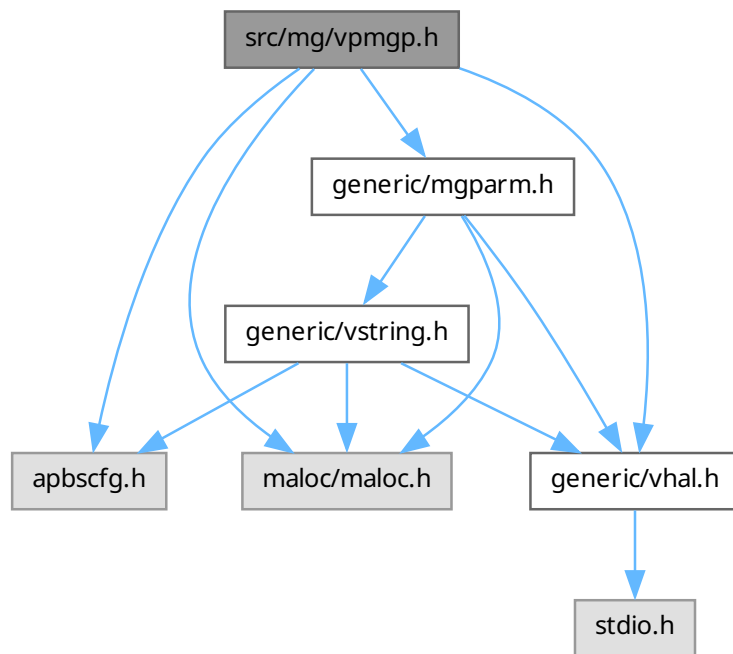
Contains declarations for class Vpmgp.

```

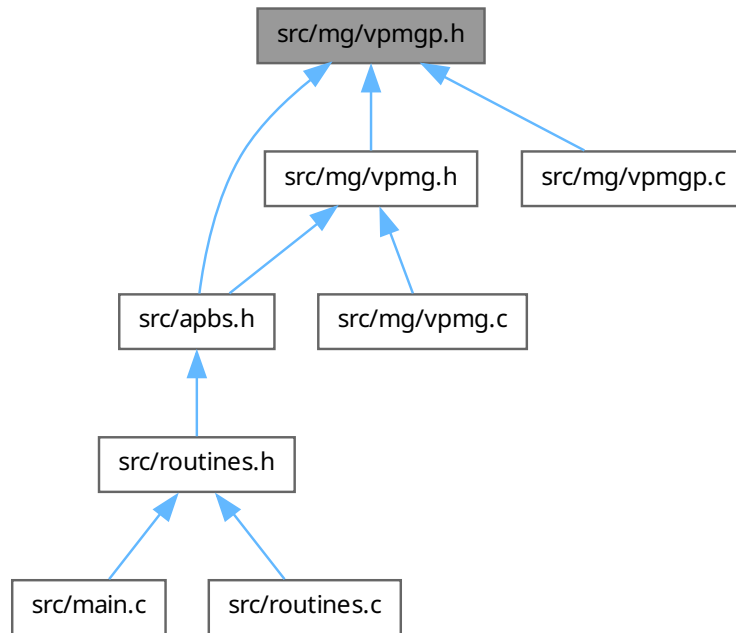
#include "apbscfg.h"
#include "maloc/maloc.h"
#include "generic/vhal.h"
#include "generic/mgparm.h"

```

Include dependency graph for `vpmgp.h`:



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [sVpmgp](#)
Contains public data members for Vpmgp class/module.

Typedefs

- typedef struct [sVpmgp](#) [Vpmgp](#)
Declaration of the Vpmgp class as the sVpmgp structure.

Functions

- VEXTERNC [Vpmgp](#) * [Vpmgp_ctor](#) ([MGparm](#) *mgparm)
Construct PMG parameter object and initialize to default values.
- VEXTERNC int [Vpmgp_ctor2](#) ([Vpmgp](#) *thee, [MGparm](#) *mgparm)
FORTTRAN stub to construct PMG parameter object and initialize to default values.
- VEXTERNC void [Vpmgp_dtor](#) ([Vpmgp](#) **thee)
Object destructor.
- VEXTERNC void [Vpmgp_dtor2](#) ([Vpmgp](#) *thee)
FORTTRAN stub for object destructor.
- VEXTERNC void [Vpmgp_size](#) ([Vpmgp](#) *thee)
Determine array sizes and parameters for multigrid solver.

- VEXTERNC void [Vpmgp_makeCoarse](#) (int numLevel, int nxOld, int nyOld, int nzOld, int *nxNew, int *nyNew, int *nzNew)

Coarsen the grid by the desired number of levels and determine the resulting numbers of grid points.

9.112.1 Detailed Description

Contains declarations for class Vpmgp.

Version

\$Id\$

Author

Nathan A. Baker

Note

Variables and many default values taken directly from PMG

Attention

```
*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
* Nathan A. Baker (nathan.baker@pnnl.gov)
* Pacific Northwest National Laboratory
*
* Additional contributing authors listed in the code documentation.
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* THE POSSIBILITY OF SUCH DAMAGE.
*
*
```

Definition in file [vpmgmp.h](#).

9.113 vpmgmp.h

[Go to the documentation of this file.](#)

```

00001
00064 #ifndef _VPMGMP_H_
00065 #define _VPMGMP_H_
00066
00067 #include "apbscfg.h"
00068
00069 #include "malloc/malloc.h"
00070
00071 #include "generic/vhal.h"
00072 #include "generic/mgparm.h"
00073
00080 struct sVpmgmp {
00081
00082     /* ***** USER-SPECIFIED PARAMETERS ***** */
00083     int nx;
00084     int ny;
00085     int nz;
00086     int nlev;
00087     double hx;
00088     double hy;
00089     double hzed;
00090     int nonlin;
00095     /* ***** DERIVED PARAMETERS ***** */
00096     int nxc;
00097     int nyc;
00098     int nzc;
00099     int nf;
00100     int nc;
00101     int narrc;
00102     int n_rpc;
00103     int n_iz;
00104     int n_ipc;
00106     size_t nrw;
00107     int niwk;
00108     int narr;
00109     int ipkey;
00117     /* ***** PARAMETERS WITH DEFAULT VALUES ***** */
00118     double xcent;
00119     double ycent;
00120     double zcent;
00121     double errtol;
00122     int itmax;
00123     int istop;
00130     int iinfo;
00135     Vbcbf bcfl;
00136     int key;
00139     int iperf;
00144     int meth;
00155     int mgkey;
00158     int nul;
00159     int nu2;
00160     int mgsmoo;
00166     int mgprol;
00170     int mgcoar;
00174     int mgsolv;
00177     int mgdisc;
00180     double omegal;
00181     double omegan;
00182     int irite;
00183     int ipcon;
00189     double xlen;
00190     double ylen;
00191     double zlen;
00192     double xmin;
00193     double ymin;
00194     double zmin;
00195     double xmax;
```

```

00196     double ymax;
00197     double zmax;
00198 };
00199
00204 typedef struct sVpmgp Vpmgp;
00205
00206 /* ////////////////////////////////////////
00207 // Class Vpmgp: Inlineable methods (vpmgp.c)
00208
00209 #if !defined(VINLINE_VPMGP)
00210 #else /* if defined(VINLINE_VPMGP) */
00212 #endif /* if !defined(VINLINE_VPMGP) */
00213
00214 /* ////////////////////////////////////////
00215 // Class Vpmgp: Non-Inlineable methods (vpmgp.c)
00216
00217 VEXTERNC Vpmgp* Vpmgp_ctor(MGparm *mgparm);
00225
00234 VEXTERNC int Vpmgp_ctor2(Vpmgp *thee, MGparm *mgparm);
00235
00241 VEXTERNC void Vpmgp_dtor(Vpmgp **thee);
00242
00248 VEXTERNC void Vpmgp_dtor2(Vpmgp *thee);
00249
00254 VEXTERNC void Vpmgp_size(
00255     Vpmgp *thee /*< Object to be sized */
00256 );
00257
00262 VEXTERNC void Vpmgp_makeCoarse(
00263     int numLevel,
00264     int nxOld,
00265     int nyOld,
00266     int nzOld,
00267     int *nxNew,
00268     int *nyNew,
00269     int *nzNew
00270 );
00271
00272
00273
00274 #endif /* ifndef _VPMGP_H_ */

```

9.114 buildAd.c

```

00001
00055 #include "buildAd.h"
00056
00057 VPUBLIC void VbuildA(int* nx, int* ny, int* nz,
00058     int* ipkey, int* mgdisc, int* numdia,
00059     int* ipc, double* rpc,
00060     double* ac, double* cc, double* fc,
00061     double* xf, double* yf, double* zf,
00062     double* gxcf, double* gycf, double* gzcf,
00063     double* alcf, double* a2cf, double* a3cf,
00064     double* ccf, double* fcf) {
00065
00066     MAT2(ac, *nx * *ny * *nz, 14);
00067
00068     if (*mgdisc == 0) {
00069
00070         VbuildA_fv(nx, ny, nz,
00071             ipkey, numdia,
00072             ipc, rpc,
00073             RAT2(ac, 1,1), cc, fc,
00074             RAT2(ac, 1,2), RAT2(ac, 1,3), RAT2(ac, 1,4),
00075             xf, yf, zf,
00076             gxcf, gycf, gzcf,
00077             alcf, a2cf, a3cf,
00078             ccf, fcf);
00079
00080     } else if (*mgdisc == 1) {
00081
00082         VbuildA_fe(nx, ny, nz,
00083             ipkey, numdia,
00084             ipc, rpc,
00085             RAT2(ac, 1, 1), cc, fc,
00086             RAT2(ac, 1, 2), RAT2(ac, 1, 3), RAT2(ac, 1, 4), RAT2(ac, 1, 5), RAT2(ac, 1, 6),
00087             RAT2(ac, 1, 7), RAT2(ac, 1, 8), RAT2(ac, 1, 9), RAT2(ac, 1,10),

```

```

00088         RAT2(ac, 1,11), RAT2(ac, 1,12), RAT2(ac, 1,13), RAT2(ac, 1,14),
00089         xf, yf, zf,
00090         gxcf, gycf, gzcf,
00091         alcf, a2cf, a3cf,
00092         ccf, fcf);
00093     } else {
00094
00095         Vnm_print(2, "VbuildA: Invalid discretization requested.\n");
00096         exit(EXIT_FAILURE);
00097     }
00098 }
00099
00100
00101
00102
00103
00104
00105 VPUBLIC void VbuildA_fv(int *nx, int *ny, int *nz,
00106     int *ipkey, int *numdia,
00107     int *ipc, double *rpc,
00108     double *oC, double *cc, double *fc, double *oE, double *oN, double *uC,
00109     double *xf, double *yf, double *zf,
00110     double *gxcf, double *gycf, double *gzcf,
00111     double *alcf, double *a2cf, double *a3cf,
00112     double *ccf, double *fcf) {
00113
00114     int i, j, k;          // @todo Document this function
00115
00116     int ike, jke, kke;
00117
00118
00119     int nxml, nym1, nzml;
00120
00121
00122
00123
00124
00125     double hx, hy, hz;
00126
00127
00128
00129
00130
00131
00132     double hxml, hym1, hzml;
00133
00134
00135     double coef_fc;
00136
00137
00138
00139     double bc_cond_e;
00140     double bc_cond_w;
00141     double bc_cond_n;
00142     double bc_cond_s;
00143     double bc_cond_u;
00144     double bc_cond_d;
00145     double coef_oE;
00146     double coef_oN;
00147     double coef_uC;
00148     double coef_oEml;
00149     double coef_oNml;
00150     double coef_uCml;
00151
00152     double diag;
00153
00154     MAT3( fc, *nx, *ny, *nz);
00155     MAT3( fcf, *nx, *ny, *nz);
00156     MAT3( cc, *nx, *ny, *nz);
00157     MAT3( ccf, *nx, *ny, *nz);
00158     MAT3( oC, *nx, *ny, *nz);
00159     MAT3(alcf, *nx, *ny, *nz);
00160     MAT3(a2cf, *nx, *ny, *nz);
00161     MAT3(a3cf, *nx, *ny, *nz);
00162     MAT3( uC, *nx, *ny, *nz);
00163     MAT3( oN, *nx, *ny, *nz);
00164     MAT3( oE, *nx, *ny, *nz);
00165     MAT3(gxcf, *ny, *nz, 2);
00166     MAT3(gycf, *nx, *nz, 2);
00167     MAT3(gzcf, *nx, *ny, 2);
00168
00169     // Save the problem key with this operator. @todo: What?
00170     VAT(ipc, 10) = *ipkey;
00171
00172     // Note how many nonzeros in this discretization stencil
00173     VAT(ipc, 11) = 7;
00174     VAT(ipc, 12) = 1;
00175     *numdia = 4;
00176
00177     // Define n and determine number of mesh points
00178     nxml = *nx - 1;
00179     nym1 = *ny - 1;

```

```

00180     nzml = *nz - 1;
00181
00182     // Determine diag scale factor
00183     // (would like something close to ones on the main diagonal)
00184     // @todo: Make a more meaningful comment
00185     diag = 1.0;
00186
00187
00188
00189     /* *****
00190     * *** interior points ***
00191     * ***** */
00192
00193     // build the operator
00194     //fprintf(data, "%s\n", PRINT_FUNC);
00195     for(k=2; k<=*nz-1; k++) {
00196
00197         hzml = VAT(zf, k) - VAT(zf, k-1);
00198         hz   = VAT(zf, k+1) - VAT(zf, k);
00199
00200         for(j=2; j<=*ny-1; j++) {
00201
00202             hyml = VAT(yf, j) - VAT(yf, j-1);
00203             hy   = VAT(yf, j+1) - VAT(yf, j);
00204
00205             for(i=2; i<=*nx-1; i++) {
00206
00207                 hxml = VAT(xf, i) - VAT(xf, i-1);
00208                 hx    = VAT(xf, i+1) - VAT(xf, i);
00209
00210                 // Calculate some coefficients
00211                 coef_oE = diag * (hyml + hy) * (hzml + hz) / (4.0 * hx);
00212                 coef_oEm1 = diag * (hyml + hy) * (hzml + hz) / (4.0 * hxml);
00213                 coef_oN = diag * (hxml + hx) * (hzml + hz) / (4.0 * hy);
00214                 coef_oNm1 = diag * (hxml + hx) * (hzml + hz) / (4.0 * hyml);
00215                 coef_uC = diag * (hxml + hx) * (hyml + hy) / (4.0 * hz);
00216                 coef_uCm1 = diag * (hxml + hx) * (hyml + hy) / (4.0 * hzml);
00217                 coef_fc = diag * (hxml + hx) * (hyml + hy) * (hzml + hz) / 8.0;
00218
00219                 // Calculate the coefficient and source function
00220                 VAT3(fc, i, j, k) = coef_fc * VAT3(fcf, i, j, k);
00221                 VAT3(cc, i, j, k) = coef_fc * VAT3(ccf, i, j, k);
00222                 //fprintf(data, "%19.12E\n", VAT3(cc, i, j, k));
00223
00224                 // Calculate the diagonal for matvecs and smoothings
00225
00226                 VAT3(oC, i, j, k) = coef_oE * VAT3(alcfc, i, j, k) +
00227                     coef_oEm1 * VAT3(alcfc, i-1, j, k) +
00228                     coef_oN * VAT3(a2cfc, i, j, k) +
00229                     coef_oNm1 * VAT3(a2cfc, i, j-1, k) +
00230                     coef_uC * VAT3(a3cfc, i, j, k) +
00231                     coef_uCm1 * VAT3(a3cfc, i, j, k-1);
00232
00233                 //fprintf(data, "%19.12E\n", VAT3(oC, i, j, k));
00234
00235                 // Calculate the east neighbor
00236                 ike = VMIN2(1, VABS(i - nxml));
00237                 VAT3(oE, i, j, k) = ike * coef_oE * VAT3(alcfc, i, j, k);
00238                 //fprintf(data, "%19.12E\n", VAT3(oE, i, j, k));
00239                 bc_cond_e = (1 - ike) * coef_oE * VAT3(alcfc, i, j, k) * VAT3(gxcfc, j, k, 2);
00240                 VAT3(fc, i, j, k) += bc_cond_e;
00241
00242                 // Calculate the north neighbor
00243                 jke = VMIN2(1, VABS(j - nym1));
00244                 VAT3(oN, i, j, k) = jke * coef_oN * VAT3(a2cfc, i, j, k);
00245                 //fprintf(data, "%19.12E\n", VAT3(oN, i, j, k));
00246                 bc_cond_n = (1 - jke) * coef_oN * VAT3(a2cfc, i, j, k) * VAT3(gycfc, i, k, 2);
00247                 VAT3(fc, i, j, k) += bc_cond_n;
00248
00249                 // Calculate the up neighbor
00250                 kke = VMIN2(1, VABS(k - nzml));
00251                 VAT3(uC, i, j, k) = kke * coef_uC * VAT3(a3cfc, i, j, k);
00252                 //fprintf(data, "%19.12E\n", VAT3(uC, i, j, k));
00253                 bc_cond_u = (1 - kke) * coef_uC * VAT3(a3cfc, i, j, k) * VAT3(gzcf, i, j, 2);
00254                 VAT3(fc, i, j, k) += bc_cond_u;
00255
00256                 // Calculate the west neighbor (just handle b.c.)
00257                 ike = VMIN2(1, VABS(i - 2));
00258                 bc_cond_w = (1 - ike) * coef_oEm1 * VAT3(alcfc, i-1, j, k) * VAT3(gxcfc, j, k, 1);
00259                 VAT3(fc, i, j, k) += bc_cond_w;
00260
00261
00262
00263
00264
00265
00266

```



```

00267         // Calculate the south neighbor (just handle b.c.)
00268         jke = VMIN2(1, VABS(j - 2));
00269         bc_cond_s = (1 - jke) * coef_oNm1 * VAT3(a2cf, i, j-1, k) * VAT3(gycf, i, k, 1);
00270         VAT3(fc, i, j, k) += bc_cond_s;
00271
00272         // Calculate the down neighbor (just handle b.c.)
00273         kke = VMIN2(1, VABS(k - 2));
00274         bc_cond_d = (1 - kke) * coef_uCm1 * VAT3(a3cf, i, j, k-1) * VAT3(gzcf, i, j, 1);
00275         VAT3(fc, i, j, k) += bc_cond_d;
00276
00277         //fprintf(data, "%19.12E\n", VAT3(fc, i, j, k));
00278     }
00279 }
00280 }
00281 }
00282
00283
00284
00285 VPUBLIC void VbuildA_fe(int *nx, int *ny, int *nz,
00286     int *ipkey, int *numdia,
00287     int *ipc, double *rpc,
00288     double *oC, double *cc, double *fc,
00289     double *oE, double *oN, double *uC,
00290     double* oNE, double* oNW,
00291     double* uE, double* uW,
00292     double* uN, double* uS,
00293     double* uNE, double* uNW, double* uSE, double* uSW,
00294     double *xf, double *yf, double *zf,
00295     double *gxcf, double *gycf, double *gzcf,
00296     double *alcf, double *a2cf, double *a3cf,
00297     double *ccf, double *fcf) {
00298     VABORT_MSG0("Untranslated Component: from buildAd.f");
00299 }

```

9.115 buildAd.h

```

00001
00049 #ifndef _VBUILD_A_H_
00050 #define _VBUILD_A_H_
00051
00052 #include "apbscfg.h"
00053
00054 #include "malloc/malloc.h"
00055
00056 #include "generic/vhal.h"
00057 #include "generic/vmatrix.h"
00058
00064 VEXTERNC void VbuildA(
00065     int* nx,
00066     int* ny,
00067     int* nz,
00068     int* ipkey,
00069     int* mgdisc,
00070     int* numdia,
00071     int* ipc,
00072     double* rpc,
00073     double* ac,
00074     double* cc,
00075     double* fc,
00076     double* xf,
00077     double* yf,
00078     double* zf,
00079     double* gxcf,
00080     double* gycf,
00081     double* gzcf,
00082     double* alcf,
00083     double* a2cf,
00084     double* a3cf,
00085     double* ccf,
00086     double* fcf
00087 );
00088
00089
00090
00161 VEXTERNC void VbuildA_fv(
00162     int* nx,
00163     int* ny,
00164     int* nz,

```

```

00165         int*    ipkey,
00166         int*    numdia,
00167         int*    ipc,
00168         double* rpc,
00169         double* oC,
00170         double* cc,
00171         double* fc,
00172         double* oE,
00173         double* oN,
00174         double* uC,
00175         double* xf,
00176         double* yf,
00177         double* zf,
00178         double* gxcf,
00179         double* gycf,
00180         double* gzcf,
00181         double* alcf,
00182         double* a2cf,
00183         double* a3cf,
00184         double* ccf,
00185         double* fcf
00186     );
00187
00188
00266 VEXTERNC void VbuildA_fe(
00267     int*    nx,
00268     int*    ny,
00269     int*    nz,
00270     int*    ipkey,
00271     int*    numdia,
00272     int*    ipc,
00273     double* rpc,
00274     double* oC,
00275     double* cc,
00276     double* fc,
00277     double* oE,
00278     double* oN,
00279     double* uC,
00280     double* oNE,
00281     double* oNW,
00282     double* uE,
00283     double* uW,
00284     double* uN,
00285     double* uS,
00286     double* uNE,
00287     double* uNW,
00288     double* uSE,
00289     double* uSW,
00290     double* xf,
00291     double* yf,
00292     double* zf,
00293     double* gxcf,
00294     double* gycf,
00295     double* gzcf,
00296     double* alcf,
00297     double* a2cf,
00298     double* a3cf,
00299     double* ccf,
00300     double* fcf
00301 );
00302
00303
00304
00305
00306
00307
00308
00309
00310
00311
00312
00313 #endif /* _VBUILD_A_H_ */

```

9.116 buildBd.c

```

00001
00055 #include "buildBd.h"
00056

```

```

00057 VPUBLIC void Vbuildband(int *key, int *nx, int *ny, int *nz,
00058     int *ipc, double *rpc, double *ac,
00059     int *ipcB, double *rpcB, double *acB) {
00060
00061     int numdia;
00062     int n, m;
00063     int lda, info;
00064
00065     MAT2(ac, *nx * *ny * *nz, 1);
00066
00067     // Do in one step
00068     numdia = VAT(ipc, 11);
00069     if (numdia == 7) {
00070
00071         n = (*nx - 2) * (*ny - 2) * (*nz - 2);
00072         m = (*nx - 2) * (*ny - 2);
00073         lda = m + 1;
00074
00075         Vbuildband1_7
00076             (nx, ny, nz,
00077             ipc, rpc,
00078             RAT2(ac, 1, 1), RAT2(ac, 1, 2), RAT2(ac, 1, 3), RAT2(ac, 1, 4),
00079             ipcB, rpcB, acB,
00080             &n, &m, &lda);
00081
00082     } else if (numdia == 27) {
00083
00084         n = (*nx - 2) * (*ny - 2) * (*nz - 2);
00085         m = (*nx - 2) * (*ny - 2) + (*nx - 2) + 1;
00086         lda = m + 1;
00087
00088         Vbuildband1_27
00089             (nx, ny, nz,
00090             ipc, rpc,
00091             RAT2(ac, 1, 1), RAT2(ac, 1, 2), RAT2(ac, 1, 3), RAT2(ac, 1, 4),
00092             RAT2(ac, 1, 5), RAT2(ac, 1, 6),
00093             RAT2(ac, 1, 7), RAT2(ac, 1, 8), RAT2(ac, 1, 9), RAT2(ac, 1, 10),
00094             RAT2(ac, 1, 11), RAT2(ac, 1, 12), RAT2(ac, 1, 13), RAT2(ac, 1, 14),
00095             ipcB, rpcB, acB,
00096             &n, &m, &lda);
00097     } else {
00098         Vnm_print(2, "Vbuildband: invalid stencil type given...");
00099     }
00100
00101     // Factor the system
00102     *key = 0;
00103     info = 0;
00104
00105     Vdgbfa(acB, &lda, &n, &m, &info);
00106     VAT(ipcB, 4) = 1;
00107
00108     if (info != 0) {
00109
00110         Vnm_print(2, "Vbuildband: dgbfa problem: %d\n", info);
00111         Vnm_print(2, "Vbuildband: leading principle minor not PD...\n");
00112
00113         *key = 1;
00114     }
00115 }
00116
00117
00118
00119 VPUBLIC void Vbuildband1_7(int *nx, int *ny, int *nz,
00120     int *ipc, double *rpc,
00121     double *oC, double *oE, double *oN, double *uC,
00122     int *ipcB, double *rpcB, double *acB,
00123     int *n, int *m, int *lda) {
00124
00125     int i, j, k;
00126     int ii, jj, kk;
00127
00128     MAT2(acB, *lda, *ny-1);
00129
00130     MAT3(oC, *nx, *ny, *nz);
00131     MAT3(oE, *nx, *ny, *nz);
00132     MAT3(oN, *nx, *ny, *nz);
00133     MAT3(uC, *nx, *ny, *nz);
00134
00135     WARN_UNTESTED;
00136
00137     // Do it

```

```

00138     VAT(ipcB, 1) = *n;
00139     VAT(ipcB, 2) = *m;
00140     VAT(ipcB, 3) = *lda;
00141     VAT(ipcB, 4) = 0;
00142
00143     jj = 0;
00144
00145     //fprintf(data, "%s\n", PRINT_FUNC);
00146
00147     for (k=2; k<=*nz-1; k++) {
00148         for (j=2; j<=*ny-1; j++) {
00149             for (i=2; i<=*nx-1; i++) {
00150                 jj++;
00151
00152                 // Diagonal term
00153                 ii = jj;
00154                 kk = ii - jj + *m + 1;
00155
00156                 VAT2(acB, kk, jj) = VAT3(oC, i, j, k);
00157
00158                 // East neighbor
00159                 ii = jj - 1;
00160                 kk = ii - jj + *m + 1;
00161                 VAT2(acB, kk, jj) = - VAT3(oE, i-1, j, k);
00162
00163                 // North neighbor
00164                 ii = jj - (*nx - 2);
00165                 kk = ii - jj + *m + 1;
00166                 VAT2(acB, kk, jj) = - VAT3(oN, i, j-1, k);
00167
00168                 // Up neighbor ***
00169                 ii = jj - (*nx - 2) * (*ny - 2);
00170                 kk = ii - jj + *m + 1;
00171                 VAT2(acB, kk, jj) = - VAT3(uC, i, j, k-1);
00172
00173                 //fprintf(data, "%19.12E\n", VAT2(acB, kk, jj));
00174             }
00175         }
00176     }
00177 }
00178 }
00179 }
00180
00181
00182
00183 VPUBLIC void Vbuildband1_27(int *nx, int *ny, int *nz,
00184     int *ipc, double *rpc,
00185     double *oC, double *oE, double *oN, double *uC,
00186     double *oNE, double *oNW,
00187     double *uE, double *uW, double *uN, double *uS,
00188     double *uNE, double *uNW, double *uSE, double *uSW,
00189     int *ipcB, double *rpcB, double *acB,
00190     int *n, int *m, int *lda) {
00191
00192     int i, j, k;
00193     int ii, jj, kk;
00194
00195     MAT2(acB, *lda, *ny-1);
00196
00197     MAT3(oC, *nx, *ny, *nz);
00198     MAT3(oE, *nx, *ny, *nz);
00199     MAT3(oN, *nx, *ny, *nz);
00200     MAT3(uC, *nx, *ny, *nz);
00201
00202     MAT3(oNE, *nx, *ny, *nz);
00203     MAT3(oNW, *nx, *ny, *nz);
00204
00205     MAT3(uE, *nx, *ny, *nz);
00206     MAT3(uW, *nx, *ny, *nz);
00207     MAT3(uN, *nx, *ny, *nz);
00208     MAT3(uS, *nx, *ny, *nz);
00209
00210     MAT3(uNE, *nx, *ny, *nz);
00211     MAT3(uNW, *nx, *ny, *nz);
00212     MAT3(uSE, *nx, *ny, *nz);
00213     MAT3(uSW, *nx, *ny, *nz);
00214
00215     // Do it
00216     VAT(ipcB, 1) = *n;
00217     VAT(ipcB, 2) = *m;
00218     VAT(ipcB, 3) = *lda;

```

```

00219     VAT(ipcB, 4) = 0;
00220
00221     jj = 0;
00222
00223     //fprintf(data, "%s\n", PRINT_FUNC);
00224
00225     for (k=2; k<=*nz-1; k++) {
00226
00227         for (j=2; j<=*ny-1; j++) {
00228
00229             for (i=2; i<=*nx-1; i++) {
00230                 jj++;
00231
00232                 // Diagonal term
00233                 ii = jj;
00234                 kk = ii - jj + *m + 1;
00235                 VAT2(acB, kk, jj) = VAT3(oC, i, j, k);
00236
00237                 // East neighbor
00238                 ii = jj - 1;
00239                 kk = ii - jj + *m + 1;
00240                 VAT2(acB, kk, jj) = - VAT3(oE, i-1, j, k);
00241
00242                 // North neighbor
00243                 ii = jj - (*nx - 2);
00244                 kk = ii - jj + *m + 1;
00245                 VAT2(acB, kk, jj) = - VAT3(oN, i, j-1, k);
00246
00247                 // North-east neighbor
00248                 ii = jj - (*nx - 2) + 1;
00249                 kk = ii - jj + *m + 1;
00250                 VAT2(acB, kk, jj) = - VAT3(oNE, i, j-1, k);
00251
00252                 // North-west neighbor
00253                 ii = jj - (*nx - 2) - 1;
00254                 kk = ii - jj + *m + 1;
00255                 VAT2(acB, kk, jj) = - VAT3(oNW, i, j-1, k);
00256
00257                 // Up neighbor
00258                 ii = jj - (*nx - 2) * (*ny - 2);
00259                 kk = ii - jj + *m + 1;
00260                 VAT2(acB, kk, jj) = - VAT3(uC, i, j, k-1);
00261
00262                 // Up-east neighbor
00263                 ii = jj - (*nx - 2) * (*ny - 2) + 1;
00264                 kk = ii - jj + *m + 1;
00265                 VAT2(acB, kk, jj) = - VAT3(uE, i, j, k-1);
00266
00267                 // Up-west neighbor
00268                 ii = jj - (*nx - 2) * (*ny - 2) - 1;
00269                 kk = ii - jj + *m + 1;
00270                 VAT2(acB, kk, jj) = - VAT3(uW, i, j, k-1);
00271
00272                 // Up-north neighbor
00273                 ii = jj - (*nx - 2) * (*ny - 2) + (*nx - 2);
00274                 kk = ii - jj + *m + 1;
00275                 VAT2(acB, kk, jj) = - VAT3(uN, i, j, k-1);
00276
00277                 // Up-south neighbor
00278                 ii = jj - (*nx - 2) * (*ny - 2) - (*nx - 2);
00279                 kk = ii - jj + *m + 1;
00280                 VAT2(acB, kk, jj) = - VAT3(uS, i, j, k-1);
00281
00282                 // Up-north-east neighbor
00283                 ii = jj - (*nx - 2) * (*ny - 2) + (*nx - 2) + 1;
00284                 kk = ii - jj + *m + 1;
00285                 VAT2(acB, kk, jj) = - VAT3(uNE, i, j, k-1);
00286
00287                 // Up-north-west neighbor
00288                 ii = jj - (*nx - 2) * (*ny - 2) + (*nx - 2) - 1;
00289                 kk = ii - jj + *m + 1;
00290                 VAT2(acB, kk, jj) = - VAT3(uNW, i, j, k-1);
00291
00292                 // Up-south-east neighbor
00293                 ii = jj - (*nx - 2) * (*ny - 2) - (*nx - 2) + 1;
00294                 kk = ii - jj + *m + 1;
00295                 VAT2(acB, kk, jj) = - VAT3(uSE, i, j, k-1);
00296
00297                 // Up-south-west neighbor
00298                 ii = jj - (*nx - 2) * (*ny - 2) - (*nx - 2) - 1;
00299                 kk = ii - jj + *m + 1;

```

```

00300             VAT2(acB, kk, jj) = - VAT3(uSW, i, j, k-1);
00301
00302             //fprintf(data, "%19.12E\n", VAT2(acB, kk, jj));
00303         }
00304     }
00305 }
00306 }

```

9.117 buildBd.h

```

00001
00049 #ifndef _BUILDBD_H_
00050 #define _BUILDBD_H_
00051
00052 #include "apbscfg.h"
00053
00054 #include "malloc/malloc.h"
00055
00056 #include "generic/vhal.h"
00057 #include "generic/vmatrix.h"
00058 #include "pmgc/mlinpckd.h"
00059
00065 VEXTERNC void Vbuildband(
00066     int *key,
00067     int *nx,
00068     int *ny,
00069     int *nz,
00070     int *ipc,
00071     double *rpc,
00072     double *aC,
00073     int *ipcB,
00074     double *rpcB,
00075     double *acB
00076 );
00077
00083 VEXTERNC void Vbuildbandl_7(
00084     int *nx,
00085     int *ny,
00086     int *nz,
00087     int *ipc,
00088     double *rpc,
00089     double *oC,
00090     double *oE,
00091     double *oN,
00092     double *uC,
00093     int *ipcB,
00094     double *rpcB,
00095     double *acB,
00096     int *n,
00097     int *m,
00098     int *lda
00099 );
00100
00106 VEXTERNC void Vbuildbandl_27(
00107     int *nx,
00108     int *ny,
00109     int *nz,
00110     int *ipc,
00111     double *rpc,
00112     double *oC,
00113     double *oE,
00114     double *oN,
00115     double *uC,
00116     double *oNE,
00117     double *oNW,
00118     double *uE,
00119     double *uW,
00120     double *uN,
00121     double *uS,
00122     double *uNE,
00123     double *uNW,
00124     double *uSE,
00125     double *uSW,
00126     int *ipcB,
00127     double *rpcB,
00128     double *acB,
00129     int *n,
00130     int *m,

```

```

00131         int *lda
00132         );
00133
00134 #endif /* _BUILDBD_H_ */

```

9.118 buildGd.c

```

00001
00055 #include "buildGd.h"
00056
00057 VPUBLIC void VbuildG(int *nxf, int *nyf, int *nzf,
00058                     int *nxc, int *nyc, int *nzc,
00059                     int *numdia,
00060                     double *pcFF, double *acFF, double *ac) {
00061
00062     MAT2(pcFF, *nxc * *nyc * *nzc, 27);
00063     MAT2(acFF, *nxf * *nyf * *nzf, 27);
00064     MAT2( ac, *nxc * *nyc * *nzc, 27);
00065
00066     // Call the build routine ***
00067     if (*numdia == 1) {
00068
00069         VbuildG_1(
00070
00071             nxf, nyf, nzf, nxc, nyc, nzc,
00072
00073             RAT2(pcFF, 1, 1), RAT2(pcFF, 1, 2), RAT2(pcFF, 1, 3), RAT2(pcFF, 1, 4), RAT2(pcFF, 1,
00074 5),
00075             RAT2(pcFF, 1, 6), RAT2(pcFF, 1, 7), RAT2(pcFF, 1, 8), RAT2(pcFF, 1, 9),
00076             RAT2(pcFF, 1, 10), RAT2(pcFF, 1, 11), RAT2(pcFF, 1, 12), RAT2(pcFF, 1, 13), RAT2(pcFF, 1,
00077 14),
00078             RAT2(pcFF, 1, 15), RAT2(pcFF, 1, 16), RAT2(pcFF, 1, 17), RAT2(pcFF, 1, 18),
00079             RAT2(pcFF, 1, 19), RAT2(pcFF, 1, 20), RAT2(pcFF, 1, 21), RAT2(pcFF, 1, 22), RAT2(pcFF, 1,
00080 23),
00081             RAT2(pcFF, 1, 24), RAT2(pcFF, 1, 25), RAT2(pcFF, 1, 26), RAT2(pcFF, 1, 27),
00082
00083             RAT2(acFF, 1, 1),
00084
00085             RAT2(ac, 1, 1), RAT2(ac, 1, 2), RAT2(ac, 1, 3),
00086             RAT2(ac, 1, 4),
00087             RAT2(ac, 1, 5), RAT2(ac, 1, 6),
00088             RAT2(ac, 1, 7), RAT2(ac, 1, 8), RAT2(ac, 1, 9), RAT2(ac, 1, 10),
00089             RAT2(ac, 1, 11), RAT2(ac, 1, 12), RAT2(ac, 1, 13), RAT2(ac, 1, 14)
00090         );
00091     } else if (*numdia == 7) {
00092
00093         VbuildG_7(
00094
00095             nxf, nyf, nzf,
00096             nxc, nyc, nzc,
00097
00098             RAT2(pcFF, 1, 1), RAT2(pcFF, 1, 2), RAT2(pcFF, 1, 3), RAT2(pcFF, 1, 4), RAT2(pcFF, 1,
00099 5),
00100             RAT2(pcFF, 1, 6), RAT2(pcFF, 1, 7), RAT2(pcFF, 1, 8), RAT2(pcFF, 1, 9),
00101             RAT2(pcFF, 1, 10), RAT2(pcFF, 1, 11), RAT2(pcFF, 1, 12), RAT2(pcFF, 1, 13), RAT2(pcFF, 1,
00102 14),
00103             RAT2(pcFF, 1, 15), RAT2(pcFF, 1, 16), RAT2(pcFF, 1, 17), RAT2(pcFF, 1, 18),
00104             RAT2(pcFF, 1, 19), RAT2(pcFF, 1, 20), RAT2(pcFF, 1, 21), RAT2(pcFF, 1, 22), RAT2(pcFF, 1,
00105 23),
00106             RAT2(pcFF, 1, 24), RAT2(pcFF, 1, 25), RAT2(pcFF, 1, 26), RAT2(pcFF, 1, 27),
00107
00108             RAT2(acFF, 1, 1), RAT2(acFF, 1, 2), RAT2(acFF, 1, 3), RAT2(acFF, 1, 4),
00109
00110             RAT2(ac, 1, 1), RAT2(ac, 1, 2), RAT2(ac, 1, 3),
00111             RAT2(ac, 1, 4),
00112             RAT2(ac, 1, 5), RAT2(ac, 1, 6),
00113             RAT2(ac, 1, 7), RAT2(ac, 1, 8), RAT2(ac, 1, 9), RAT2(ac, 1, 10),
00114             RAT2(ac, 1, 11), RAT2(ac, 1, 12), RAT2(ac, 1, 13), RAT2(ac, 1, 14)
00115         );
00116     } else if (*numdia == 27) {
00117
00118         VbuildG_27(
00119
00120             nxf, nyf, nzf,

```

```

00119         nxc, nyc, nzc,
00120
00121         RAT2(pcFF, 1, 1), RAT2(pcFF, 1, 2), RAT2(pcFF, 1, 3), RAT2(pcFF, 1, 4), RAT2(pcFF, 1,
5),
00122         RAT2(pcFF, 1, 6), RAT2(pcFF, 1, 7), RAT2(pcFF, 1, 8), RAT2(pcFF, 1, 9),
00123         RAT2(pcFF, 1, 10), RAT2(pcFF, 1, 11), RAT2(pcFF, 1, 12), RAT2(pcFF, 1, 13), RAT2(pcFF, 1,
14),
00124         RAT2(pcFF, 1, 15), RAT2(pcFF, 1, 16), RAT2(pcFF, 1, 17), RAT2(pcFF, 1, 18),
00125         RAT2(pcFF, 1, 19), RAT2(pcFF, 1, 20), RAT2(pcFF, 1, 21), RAT2(pcFF, 1, 22), RAT2(pcFF, 1,
23),
00126         RAT2(pcFF, 1, 24), RAT2(pcFF, 1, 25), RAT2(pcFF, 1, 26), RAT2(pcFF, 1, 27),
00127
00128         RAT2(acFF, 1, 1), RAT2(acFF, 1, 2), RAT2(acFF, 1, 3), RAT2(acFF, 1, 4),
00129         RAT2(acFF, 1, 5), RAT2(acFF, 1, 6), RAT2(acFF, 1, 7), RAT2(acFF, 1, 8), RAT2(acFF, 1,
9),
00130         RAT2(acFF, 1, 10), RAT2(acFF, 1, 11), RAT2(acFF, 1, 12), RAT2(acFF, 1, 13), RAT2(acFF, 1,
14),
00131
00132         RAT2(ac, 1, 1), RAT2(ac, 1, 2), RAT2(ac, 1, 3),
00133         RAT2(ac, 1, 4),
00134         RAT2(ac, 1, 5), RAT2(ac, 1, 6),
00135         RAT2(ac, 1, 7), RAT2(ac, 1, 8), RAT2(ac, 1, 9), RAT2(ac, 1, 10),
00136         RAT2(ac, 1, 11), RAT2(ac, 1, 12), RAT2(ac, 1, 13), RAT2(ac, 1, 14)
00137     );
00138 }
00139 } else {
00140     Vnm_print(2, "BUILDG: invalid stencil type given...\n");
00141 }
00142 }
00143 }
00144
00145 VPUBLIC void VbuildG_1(int *nxf, int *nyf, int *nzf,
00146     int *nx, int *ny, int *nz,
00147     double *oPC, double *oPN, double *oPS, double *oPE, double *oPW,
00148     double *oPNE, double *oPNW, double *oPSE, double *oPSW,
00149     double *uPC, double *uPN, double *uPS, double *uPE, double *uPW,
00150     double *uPNE, double *uPNW, double *uPSE, double *uPSW,
00151     double *dPC, double *dPN, double *dPS, double *dPE, double *dPW,
00152     double *dPNE, double *dPNW, double *dPSE, double *dPSW,
00153     double *oC,
00154     double *XoC, double *XoE, double *XoN,
00155     double *XuC,
00156     double *XoNE, double *XoNW,
00157     double *XuE, double *XuW, double *XuN, double *XuS,
00158     double *XuNE, double *XuNW, double *XuSE, double *XuSW
00159 ) {
00160
00161     int i, j, k, ii, jj, kk;
00162     int im1, ip1, jm1, jp1, km1, kp1;
00163     int iim1, iip1, jjm1, jjp1, kkm1, kkp1;
00164     int nxm1, nym1, nzm1;
00165
00166     double TMP1_XOC, TMP2_XOC, TMP3_XOC;
00167
00168     MAT3( oC, *nxf, *nyf, *nzf);
00169
00170     MAT3( XoC, *nx, *ny, *nz);
00171     MAT3( XoE, *nx, *ny, *nz);
00172     MAT3( XoN, *nx, *ny, *nz);
00173
00174     MAT3( XuC, *nx, *ny, *nz);
00175
00176     MAT3( XoNE, *nx, *ny, *nz);
00177     MAT3( XoNW, *nx, *ny, *nz);
00178
00179     MAT3( XuE, *nx, *ny, *nz);
00180     MAT3( XuW, *nx, *ny, *nz);
00181     MAT3( XuN, *nx, *ny, *nz);
00182     MAT3( XuS, *nx, *ny, *nz);
00183     MAT3( XuNE, *nx, *ny, *nz);
00184     MAT3( XuNW, *nx, *ny, *nz);
00185     MAT3( XuSE, *nx, *ny, *nz);
00186     MAT3( XuSW, *nx, *ny, *nz);
00187
00188     MAT3( oPC, *nx, *ny, *nz);
00189     MAT3( oPN, *nx, *ny, *nz);
00190     MAT3( oPS, *nx, *ny, *nz);
00191     MAT3( oPE, *nx, *ny, *nz);
00192     MAT3( oPW, *nx, *ny, *nz);
00193     MAT3( oPNE, *nx, *ny, *nz);
00194     MAT3( oPNW, *nx, *ny, *nz);

```



```

00195     MAT3(oPSE, *nx, *ny, *nz);
00196     MAT3(oPSW, *nx, *ny, *nz);
00197
00198     MAT3(uPC, *nx, *ny, *nz);
00199     MAT3(uPN, *nx, *ny, *nz);
00200     MAT3(uPS, *nx, *ny, *nz);
00201     MAT3(uPE, *nx, *ny, *nz);
00202     MAT3(uPW, *nx, *ny, *nz);
00203     MAT3(uPNE, *nx, *ny, *nz);
00204     MAT3(uPNW, *nx, *ny, *nz);
00205     MAT3(uPSE, *nx, *ny, *nz);
00206     MAT3(uPSW, *nx, *ny, *nz);
00207
00208     MAT3(dPC, *nx, *ny, *nz);
00209     MAT3(dPN, *nx, *ny, *nz);
00210     MAT3(dPS, *nx, *ny, *nz);
00211     MAT3(dPE, *nx, *ny, *nz);
00212     MAT3(dPW, *nx, *ny, *nz);
00213     MAT3(dPNE, *nx, *ny, *nz);
00214     MAT3(dPNW, *nx, *ny, *nz);
00215     MAT3(dPSE, *nx, *ny, *nz);
00216     MAT3(dPSW, *nx, *ny, *nz);
00217
00218     // Define n and determine number of mesh points
00219     nxm1 = *nx - 1;
00220     nym1 = *ny - 1;
00221     nzm1 = *nz - 1;
00222
00223     //fprintf(data, "%s\n", PRINT_FUNC);
00224
00225     // Build the operator
00226     for(kk=2; kk<=*nz-1; kk++) {
00227         k = 2 * kk - 1;
00228
00229         for(jj=2; jj<=*ny-1; jj++) {
00230             j = 2 * jj - 1;
00231
00232             for(ii=2; ii<=*nx-1; ii++) {
00233                 i = 2 * ii - 1;
00234
00235                 // Index computations
00236                 im1 = i - 1;
00237                 ip1 = i + 1;
00238                 jm1 = j - 1;
00239                 jp1 = j + 1;
00240                 km1 = k - 1;
00241                 kp1 = k + 1;
00242                 iim1 = ii - 1;
00243                 iip1 = ii + 1;
00244                 jjm1 = jj - 1;
00245                 jjp1 = jj + 1;
00246                 kkm1 = kk - 1;
00247                 kkp1 = kk + 1;
00248
00249                 /* *****
00250                  * oC
00251                  * *****
00252
00253                 // XoC(ii,jj,kk) =
00254                 TMP1_XOC =
00255                     VAT3(uPS, ii, jj, kk) * VAT3(uPS, ii, jj, kk) * VAT3(oC, i, jm1, kp1)
00256                     + VAT3(dPSW, ii, jj, kk) * VAT3(dPSW, ii, jj, kk) * VAT3(oC, im1, jm1, km1)
00257                     + VAT3(oPSW, ii, jj, kk) * VAT3(oPSW, ii, jj, kk) * VAT3(oC, im1, jm1, k)
00258                     + VAT3(uPSW, ii, jj, kk) * VAT3(uPSW, ii, jj, kk) * VAT3(oC, im1, jm1, kp1)
00259                     + VAT3(dPW, ii, jj, kk) * VAT3(dPW, ii, jj, kk) * VAT3(oC, im1, j, km1)
00260                     + VAT3(oPW, ii, jj, kk) * VAT3(oPW, ii, jj, kk) * VAT3(oC, im1, j, k)
00261                     + VAT3(uPNW, ii, jj, kk) * VAT3(uPNW, ii, jj, kk) * VAT3(oC, im1, jp1, kp1)
00262                     + VAT3(dPS, ii, jj, kk) * VAT3(dPS, ii, jj, kk) * VAT3(oC, i, jm1, km1)
00263                     + VAT3(oPS, ii, jj, kk) * VAT3(oPS, ii, jj, kk) * VAT3(oC, i, jm1, k);
00264
00265                 TMP2_XOC =
00266                     VAT3(dPC, ii, jj, kk) * VAT3(dPC, ii, jj, kk) * VAT3(oC, i, j, km1)
00267                     + VAT3(oPC, ii, jj, kk) * VAT3(oPC, ii, jj, kk) * VAT3(oC, i, j, k)
00268                     + VAT3(uPC, ii, jj, kk) * VAT3(uPC, ii, jj, kk) * VAT3(oC, i, j, kp1)
00269                     + VAT3(dPN, ii, jj, kk) * VAT3(dPN, ii, jj, kk) * VAT3(oC, i, jp1, km1)
00270                     + VAT3(oPN, ii, jj, kk) * VAT3(oPN, ii, jj, kk) * VAT3(oC, i, jp1, k)
00271                     + VAT3(uPW, ii, jj, kk) * VAT3(uPW, ii, jj, kk) * VAT3(oC, im1, j, kp1)
00272                     + VAT3(dPNW, ii, jj, kk) * VAT3(dPNW, ii, jj, kk) * VAT3(oC, im1, jp1, km1)
00273                     + VAT3(oPNW, ii, jj, kk) * VAT3(oPNW, ii, jj, kk) * VAT3(oC, im1, jp1, k)
00274                     + VAT3(oPE, ii, jj, kk) * VAT3(oPE, ii, jj, kk) * VAT3(oC, ip1, j, k);
00275

```

```

00276     TMP3_XOC =
00277         VAT3( uPE, ii,jj,kk) * VAT3( uPE, ii,jj,kk) * VAT3( oC, ip1,j,kp1)
00278     + VAT3( dPNE, ii,jj,kk) * VAT3( dPNE, ii,jj,kk) * VAT3( oC, ip1,jp1,kml)
00279     + VAT3( oPNE, ii,jj,kk) * VAT3( oPNE, ii,jj,kk) * VAT3( oC, ip1,jp1,k)
00280     + VAT3( uPNE, ii,jj,kk) * VAT3( uPNE, ii,jj,kk) * VAT3( oC, ip1,jp1,kp1)
00281     + VAT3( uPN, ii,jj,kk) * VAT3( uPN, ii,jj,kk) * VAT3( oC, i,jp1,kp1)
00282     + VAT3( dPSE, ii,jj,kk) * VAT3( dPSE, ii,jj,kk) * VAT3( oC, ip1,jml,kml)
00283     + VAT3( oPSE, ii,jj,kk) * VAT3( oPSE, ii,jj,kk) * VAT3( oC, ip1,jml,k)
00284     + VAT3( uPSE, ii,jj,kk) * VAT3( uPSE, ii,jj,kk) * VAT3( oC, ip1,jml,kp1)
00285     + VAT3( dPE, ii,jj,kk) * VAT3( dPE, ii,jj,kk) * VAT3( oC, ip1,j,kml);
00286
00287     VAT3( XoC, ii,jj,kk) = TMP1_XOC + TMP2_XOC + TMP3_XOC;
00288
00289     //fprintf(data, "%19.12E\n", VAT3(XoC, ii, jj, kk));
00290
00291     /* *****
00292     * *** > oE;
00293     * *****/
00294
00295     VAT3( XoE, ii,jj,kk) =
00296         - VAT3( dPSE, ii,jj,kk) * VAT3( oC, ip1,jml,kml) * VAT3( dPSW, iip1,jj,kk)
00297         - VAT3( oPSE, ii,jj,kk) * VAT3( oC, ip1,jml,k) * VAT3( oPSW, iip1,jj,kk)
00298         - VAT3( uPSE, ii,jj,kk) * VAT3( oC, ip1,jml,kp1) * VAT3( uPSW, iip1,jj,kk)
00299         - VAT3( dPE, ii,jj,kk) * VAT3( oC, ip1,j,kml) * VAT3( dPW, iip1,jj,kk)
00300         - VAT3( oPE, ii,jj,kk) * VAT3( oC, ip1,j,k) * VAT3( oPW, iip1,jj,kk)
00301         - VAT3( uPE, ii,jj,kk) * VAT3( oC, ip1,j,kp1) * VAT3( uPW, iip1,jj,kk)
00302         - VAT3( dPNE, ii,jj,kk) * VAT3( oC, ip1,jp1,kml) * VAT3( dPNW, iip1,jj,kk)
00303         - VAT3( oPNE, ii,jj,kk) * VAT3( oC, ip1,jp1,k) * VAT3( oPNW, iip1,jj,kk)
00304         - VAT3( uPNE, ii,jj,kk) * VAT3( oC, ip1,jp1,kp1) * VAT3( uPNW, iip1,jj,kk);
00305
00306     //fprintf(data, "%19.12E\n", VAT3(XoE, ii, jj, kk));
00307
00308     /* *****
00309     * *** > oN;
00310     * *****/
00311
00312     VAT3( XoN, ii,jj,kk) =
00313         - VAT3( dPNW, ii,jj,kk) * VAT3( oC, im1,jp1,kml) * VAT3( dPSW, ii,jjp1,kk)
00314         - VAT3( oPNW, ii,jj,kk) * VAT3( oC, im1,jp1,k) * VAT3( oPSW, ii,jjp1,kk)
00315         - VAT3( uPNW, ii,jj,kk) * VAT3( oC, im1,jp1,kp1) * VAT3( uPSW, ii,jjp1,kk)
00316         - VAT3( dPN, ii,jj,kk) * VAT3( oC, i,jp1,kml) * VAT3( dPS, ii,jjp1,kk)
00317         - VAT3( oPN, ii,jj,kk) * VAT3( oC, i,jp1,k) * VAT3( oPS, ii,jjp1,kk)
00318         - VAT3( uPN, ii,jj,kk) * VAT3( oC, i,jp1,kp1) * VAT3( uPS, ii,jjp1,kk)
00319         - VAT3( dPNE, ii,jj,kk) * VAT3( oC, ip1,jp1,kml) * VAT3( dPSE, ii,jjp1,kk)
00320         - VAT3( oPNE, ii,jj,kk) * VAT3( oC, ip1,jp1,k) * VAT3( oPSE, ii,jjp1,kk)
00321         - VAT3( uPNE, ii,jj,kk) * VAT3( oC, ip1,jp1,kp1) * VAT3( uPSE, ii,jjp1,kk);
00322
00323     //fprintf(data, "%19.12E\n", VAT3(XoN, ii, jj, kk));
00324
00325     /* *****
00326     * *** > uC;
00327     * *****/
00328
00329     VAT3( XuC, ii,jj,kk) =
00330         - VAT3( dPSW, ii,jj,kkp1) * VAT3( oC, im1,jml,kp1) * VAT3( uPSW, ii,jj,kk)
00331         - VAT3( dPW, ii,jj,kkp1) * VAT3( oC, im1,j,kp1) * VAT3( uPW, ii,jj,kk)
00332         - VAT3( dPNW, ii,jj,kkp1) * VAT3( oC, im1,jp1,kp1) * VAT3( uPNW, ii,jj,kk)
00333         - VAT3( dPS, ii,jj,kkp1) * VAT3( oC, i,jml,kp1) * VAT3( uPS, ii,jj,kk)
00334         - VAT3( dPC, ii,jj,kkp1) * VAT3( oC, i,j,kp1) * VAT3( uPC, ii,jj,kk)
00335         - VAT3( dPN, ii,jj,kkp1) * VAT3( oC, i,jp1,kp1) * VAT3( uPN, ii,jj,kk)
00336         - VAT3( dPSE, ii,jj,kkp1) * VAT3( oC, ip1,jml,kp1) * VAT3( uPSE, ii,jj,kk)
00337         - VAT3( dPE, ii,jj,kkp1) * VAT3( oC, ip1,j,kp1) * VAT3( uPE, ii,jj,kk)
00338         - VAT3( dPNE, ii,jj,kkp1) * VAT3( oC, ip1,jp1,kp1) * VAT3( uPNE, ii,jj,kk);
00339
00340     //fprintf(data, "%19.12E\n", VAT3(XuC, ii, jj, kk));
00341
00342     /* *****
00343     * *** > oNE;
00344     * *****/
00345
00346     VAT3( XoNE, ii,jj,kk) =
00347         - VAT3( dPNE, ii,jj,kk) * VAT3( oC, ip1,jp1,kml) * VAT3( dPSW, iip1,jjp1,kk)
00348         - VAT3( oPNE, ii,jj,kk) * VAT3( oC, ip1,jp1,k) * VAT3( oPSW, iip1,jjp1,kk)
00349         - VAT3( uPNE, ii,jj,kk) * VAT3( oC, ip1,jp1,kp1) * VAT3( uPSW, iip1,jjp1,kk);
00350
00351     //fprintf(data, "%19.12E\n", VAT3(XoNE, ii, jj, kk));
00352
00353     /* *****
00354     * *** > oNW;
00355     * *****/
00356

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00357
00358 VAT3(XoNW, ii,jj,kk) =
00359     - VAT3(dPNW, ii,jj,kk) * VAT3( oC, iml,jpl,kml) * VAT3(dPSE, iiml,jjpl,kk)
00360     - VAT3(oPNW, ii,jj,kk) * VAT3( oC, iml,jpl,k) * VAT3(oPSE, iiml,jjpl,kk)
00361     - VAT3(uPNW, ii,jj,kk) * VAT3( oC, iml,jpl,kpl) * VAT3(uPSE, iiml,jjpl,kk);
00362
00363 //fprintf(data, "%19.12E\n", VAT3(XoNW, ii, jj, kk));
00364
00365 /* *****
00366 * *** > uE;
00367 * *****/
00368
00369 VAT3( XuE, ii,jj,kk) =
00370     - VAT3(uPSE, ii,jj,kk) * VAT3( oC, ip1,jml,kpl) * VAT3(dPSW, iip1,jj,kkp1)
00371     - VAT3( uPE, ii,jj,kk) * VAT3( oC, ip1,j,kpl) * VAT3( dPW, iip1,jj,kkp1)
00372     - VAT3(uPNE, ii,jj,kk) * VAT3( oC, ip1,jpl,kpl) * VAT3(dPNW, iip1,jj,kkp1);
00373
00374 //fprintf(data, "%19.12E\n", VAT3(XuE, ii, jj, kk));
00375
00376 /* *****
00377 * *** > uW;
00378 * *****/
00379
00380 VAT3( XuW, ii,jj,kk) =
00381     - VAT3(uPSW, ii,jj,kk) * VAT3( oC, iml,jml,kpl) * VAT3(dPSE, iiml,jj,kkp1)
00382     - VAT3( uPW, ii,jj,kk) * VAT3( oC, iml,j,kpl) * VAT3( dPE, iiml,jj,kkp1)
00383     - VAT3(uPNW, ii,jj,kk) * VAT3( oC, iml,jpl,kpl) * VAT3(dPNE, iiml,jj,kkp1);
00384
00385 //fprintf(data, "%19.12E\n", VAT3(XuW, ii, jj, kk));
00386
00387 /* *****
00388 * *** > uN;
00389 * *****/
00390
00391 VAT3( XuN, ii,jj,kk) =
00392     - VAT3(uPNW, ii,jj,kk) * VAT3( oC, iml,jpl,kpl) * VAT3(dPSW, ii,jjpl,kkp1)
00393     - VAT3( uPN, ii,jj,kk) * VAT3( oC, i,jpl,kpl) * VAT3( dPS, ii,jjpl,kkp1)
00394     - VAT3(uPNE, ii,jj,kk) * VAT3( oC, ip1,jpl,kpl) * VAT3(dPSE, ii,jjpl,kkp1);
00395
00396 //fprintf(data, "%19.12E\n", VAT3(XuN, ii, jj, kk));
00397
00398 /* *****
00399 * *** > uS;
00400 * *****/
00401
00402 VAT3( XuS, ii,jj,kk) =
00403     - VAT3(uPSW, ii,jj,kk) * VAT3( oC, iml,jml,kpl) * VAT3(dPNW, ii,jjml,kkp1)
00404     - VAT3( uPS, ii,jj,kk) * VAT3( oC, i,jml,kpl) * VAT3( dPN, ii,jjml,kkp1)
00405     - VAT3(uPSE, ii,jj,kk) * VAT3( oC, ip1,jml,kpl) * VAT3(dPNE, ii,jjml,kkp1);
00406
00407 //fprintf(data, "%19.12E\n", VAT3(XuS, ii, jj, kk));
00408
00409 /* *****
00410 * *** > uNE;
00411 * *****/
00412
00413 VAT3(XuNE, ii,jj,kk) =
00414     - VAT3(uPNE, ii,jj,kk) * VAT3( oC, ip1,jpl,kpl) * VAT3(dPSW, iip1,jjpl,kkp1);
00415
00416 //fprintf(data, "%19.12E\n", VAT3(XuNE, ii, jj, kk));
00417
00418 /* *****
00419 * *** > uNW;
00420 * *****/
00421
00422 VAT3(XuNW, ii,jj,kk) =
00423     - VAT3(uPNW, ii,jj,kk) * VAT3( oC, iml,jpl,kpl) * VAT3(dPSE, iiml,jjpl,kkp1);
00424
00425 //fprintf(data, "%19.12E\n", VAT3(XuNW, ii, jj, kk));
00426
00427 /* *****
00428 * *** > uSE;
00429 * *****/
00430
00431 VAT3(XuSE, ii,jj,kk) =
00432     - VAT3(uPSE, ii,jj,kk) * VAT3( oC, ip1,jml,kpl) * VAT3(dPNW, iip1,jjml,kkp1);
00433
00434 //fprintf(data, "%19.12E\n", VAT3(XuSE, ii, jj, kk));
00435
00436 /* *****
00437 * *** > uSW;

```

```

00438          * *****/
00439
00440      VAT3(XuSW, ii,jj,kk) =
00441          - VAT3(uPSW, ii,jj,kk) * VAT3( oC, im1,jm1,kp1) * VAT3(dPNE, iim1,jjm1,kkp1);
00442
00443      //fprintf(data, "%19.12E\n", VAT3(XuSW, ii, jj, kk));
00444
00445      }
00446  }
00447 }
00448 }
00449
00450 VPUBLIC void VbuildG_7(int *nxf, int *nyf, int *nzf,
00451      int *nx, int *ny, int *nz,
00452      double *oPC, double *oPN, double *oPS, double *oPE, double *oPW,
00453      double *oPNE, double *oPNW, double *oPSE, double *oPSW,
00454      double *uPC, double *uPN, double *uPS, double *uPE, double *uPW,
00455      double *uPNE, double *uPNW, double *uPSE, double *uPSW,
00456      double *dPC, double *dPN, double *dPS, double *dPE, double *dPW,
00457      double *dPNE, double *dPNW, double *dPSE, double *dPSW,
00458      double *oC, double *oE, double *oN, double *uC,
00459      double *XoC, double *XoE, double *XoN,
00460      double *XuC,
00461      double *XoNE, double *XoNW,
00462      double *XuE, double *XuW, double *XuN, double *XuS,
00463      double *XuNE, double *XuNW, double *XuSE, double *XuSW) {
00464
00465      int i, j, k;
00466      int ii, jj, kk;
00467      int im1, ip1, im2, ip2;
00468      int jm1, jp1, jm2, jp2;
00469      int km1, kp1, km2, kp2;
00470      int iim1, iip1;
00471      int jjm1, jjp1;
00472      int kkm1, kkp1;
00473      int nxm1, nym1, nzm1;
00474
00475      double TMP1_XOC, TMP2_XOC, TMP3_XOC, TMP4_XOC;
00476      double TMP5_XOC, TMP6_XOC, TMP7_XOC, TMP8_XOC;
00477      double TMP9_XOC;
00478      double TMP1_XOE, TMP2_XOE, TMP3_XOE, TMP4_XOE;
00479      double TMP1_XON, TMP2_XON, TMP3_XON, TMP4_XON;
00480      double TMP1_XUC, TMP2_XUC, TMP3_XUC, TMP4_XUC;
00481
00482      MAT3( oC, *nxf, *nyf, *nzf);
00483      MAT3( oE, *nxf, *nyf, *nzf);
00484      MAT3( oN, *nxf, *nyf, *nzf);
00485
00486      MAT3( uC, *nxf, *nyf, *nzf);
00487
00488      MAT3( XoC, *nx, *ny, *nz);
00489      MAT3( XoE, *nx, *ny, *nz);
00490      MAT3( XoN, *nx, *ny, *nz);
00491      MAT3(XoNE, *nx, *ny, *nz);
00492      MAT3(XoNW, *nx, *ny, *nz);
00493
00494      MAT3( XuC, *nx, *ny, *nz);
00495      MAT3( XuE, *nx, *ny, *nz);
00496      MAT3( XuW, *nx, *ny, *nz);
00497      MAT3( XuN, *nx, *ny, *nz);
00498      MAT3( XuS, *nx, *ny, *nz);
00499      MAT3(XuNE, *nx, *ny, *nz);
00500      MAT3(XuNW, *nx, *ny, *nz);
00501      MAT3(XuSE, *nx, *ny, *nz);
00502      MAT3(XuSW, *nx, *ny, *nz);
00503
00504      MAT3( oPC, *nx, *ny, *nz);
00505      MAT3( oPN, *nx, *ny, *nz);
00506      MAT3( oPS, *nx, *ny, *nz);
00507      MAT3( oPE, *nx, *ny, *nz);
00508      MAT3( oPW, *nx, *ny, *nz);
00509      MAT3(oPNE, *nx, *ny, *nz);
00510      MAT3(oPNW, *nx, *ny, *nz);
00511      MAT3(oPSE, *nx, *ny, *nz);
00512      MAT3(oPSW, *nx, *ny, *nz);
00513
00514      MAT3( uPC, *nx, *ny, *nz);
00515      MAT3( uPN, *nx, *ny, *nz);
00516      MAT3( uPS, *nx, *ny, *nz);
00517      MAT3( uPE, *nx, *ny, *nz);
00518      MAT3( uPW, *nx, *ny, *nz);

```

```

00519     MAT3(uPNE, *nx, *ny, *nz);
00520     MAT3(uPNW, *nx, *ny, *nz);
00521     MAT3(uPSE, *nx, *ny, *nz);
00522     MAT3(uPSW, *nx, *ny, *nz);
00523
00524     MAT3(dPC, *nx, *ny, *nz);
00525     MAT3(dPN, *nx, *ny, *nz);
00526     MAT3(dPS, *nx, *ny, *nz);
00527     MAT3(dPE, *nx, *ny, *nz);
00528     MAT3(dPW, *nx, *ny, *nz);
00529     MAT3(dPNE, *nx, *ny, *nz);
00530     MAT3(dPNW, *nx, *ny, *nz);
00531     MAT3(dPSE, *nx, *ny, *nz);
00532     MAT3(dPSW, *nx, *ny, *nz);
00533
00534     // Define n and determine number of mesh points
00535     nxm1 = *nx - 1;
00536     nym1 = *ny - 1;
00537     nzm1 = *nz - 1;
00538
00539     //fprintf(data, "%s\n", PRINT_FUNC);
00540
00541     // Build the operator ***
00542     for(kk=2; kk<=*nz-1; kk++) {
00543         k = 2 * kk - 1;
00544
00545         for(jj=2; jj<=*ny-1; jj++) {
00546             j = 2 * jj - 1;
00547
00548             for(ii=2; ii<=*nx-1; ii++) {
00549                 i = 2 * ii - 1;
00550
00551                 // Index computations
00552                 im1 = i - 1;
00553                 ip1 = i + 1;
00554                 im2 = i - 2;
00555                 ip2 = i + 2;
00556                 jm1 = j - 1;
00557                 jp1 = j + 1;
00558                 jm2 = j - 2;
00559                 jp2 = j + 2;
00560                 km1 = k - 1;
00561                 kp1 = k + 1;
00562                 km2 = k - 2;
00563                 kp2 = k + 2;
00564                 iim1 = ii - 1;
00565                 iip1 = ii + 1;
00566                 jjm1 = jj - 1;
00567                 jjp1 = jj + 1;
00568                 kkm1 = kk - 1;
00569                 kkp1 = kk + 1;
00570
00571                 /* *****
00572                 * *** > oC;
00573                 * *****/
00574
00575                 // XoC(ii,jj,kk) =
00576                 TMP1_XOC =
00577                     VAT3(dPSW, ii,jj,kk) * ( VAT3(oC, im1,jm1,km1) * VAT3(dPSW, ii,jj,kk)
00578                         - VAT3(uC, im1,jm1,km1) * VAT3(oPSW, ii,jj,kk)
00579                         - VAT3(oN, im1,jm1,km1) * VAT3(dPW, ii,jj,kk)
00580                         - VAT3(oE, im1,jm1,km1) * VAT3(dPS, ii,jj,kk))
00581
00582                     + VAT3(oPNE, ii,jj,kk) * (- VAT3(oE, i,jp1, k) * VAT3(oPN, ii,jj,kk)
00583                         - VAT3(oN, ip1, j, k) * VAT3(oPE, ii,jj,kk)
00584                         - VAT3(uC, ip1,jp1,km1) * VAT3(dPNE, ii,jj,kk)
00585                         + VAT3(oC, ip1,jp1, k) * VAT3(oPNE, ii,jj,kk)
00586                         - VAT3(uC, ip1,jp1, k) * VAT3(uPNE, ii,jj,kk))
00587
00588                     + VAT3(dPNE, ii,jj,kk) * (- VAT3(oE, i,jp1,km1) * VAT3(dPN, ii,jj,kk)
00589                         - VAT3(oN, ip1, j,km1) * VAT3(dPE, ii,jj,kk)
00590                         + VAT3(oC, ip1,jp1,km1) * VAT3(dPNE, ii,jj,kk)
00591                         - VAT3(uC, ip1,jp1,km1) * VAT3(oPNE, ii,jj,kk));
00592
00593                 TMP2_XOC =
00594                     VAT3(dPSE, ii,jj,kk) * (- VAT3(oE, i,jm1,km1) * VAT3(dPS, ii,jj,kk)
00595                         + VAT3(oC, ip1,jm1,km1) * VAT3(dPSE, ii,jj,kk)
00596                         - VAT3(uC, ip1,jm1,km1) * VAT3(oPSE, ii,jj,kk)
00597                         - VAT3(oN, ip1,jm1,km1) * VAT3(dPE, ii,jj,kk))
00598
00599                     + VAT3(uPE, ii,jj,kk) * (- VAT3(oE, i, j,kp1) * VAT3(uPC, ii,jj,kk)

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00600             - VAT3( oN, ip1,jm1,kp1) * VAT3(uPSE, ii,jj,kk)
00601             - VAT3( uC, ip1, j, k) * VAT3( oPE, ii,jj,kk)
00602             + VAT3( oC, ip1, j,kp1) * VAT3( uPE, ii,jj,kk)
00603             - VAT3( oN, ip1, j,kp1) * VAT3(uPNE, ii,jj,kk))
00604
00605             + VAT3( oPE, ii,jj,kk) * (- VAT3( oE, i, j, k) * VAT3( oPC, ii,jj,kk)
00606             - VAT3( oN, ip1,jm1, k) * VAT3(oPSE, ii,jj,kk)
00607             - VAT3( uC, ip1, j,kml) * VAT3( dPE, ii,jj,kk)
00608             + VAT3( oC, ip1, j, k) * VAT3( oPE, ii,jj,kk)
00609             - VAT3( uC, ip1, j, k) * VAT3( uPE, ii,jj,kk)
00610             - VAT3( oN, ip1, j, k) * VAT3(oPNE, ii,jj,kk));
00611
00612 TMP3_XOC =
00613             + VAT3( dPE, ii,jj,kk) * (- VAT3( oE, i, j,kml) * VAT3( dPC, ii,jj,kk)
00614             - VAT3( oN, ip1,jm1,kml) * VAT3(dPSE, ii,jj,kk)
00615             + VAT3( oC, ip1, j,kml) * VAT3( dPE, ii,jj,kk)
00616             - VAT3( uC, ip1, j,kml) * VAT3( oPE, ii,jj,kk)
00617             - VAT3( oN, ip1, j, kml) * VAT3( dPNE, ii,jj,kk))
00618
00619             + VAT3(uPSE, ii,jj,kk) * (- VAT3( oE, i,jm1,kp1) * VAT3( uPS, ii,jj,kk)
00620             - VAT3( uC, ip1,jm1, k) * VAT3(oPSE, ii,jj,kk)
00621             + VAT3( oC, ip1,jm1,kp1) * VAT3(uPSE, ii,jj,kk)
00622             - VAT3( oN, ip1,jm1,kp1) * VAT3( uPE, ii,jj,kk))
00623
00624             + VAT3(uPNE, ii,jj,kk) * (- VAT3( oE, i,jp1,kp1) * VAT3( uPN, ii,jj,kk)
00625             - VAT3( oN, ip1, j,kp1) * VAT3( uPE, ii,jj,kk)
00626             - VAT3( uC, ip1,jp1, k) * VAT3(oPNE, ii,jj,kk)
00627             + VAT3( oC, ip1,jp1,kp1) * VAT3(uPNE, ii,jj,kk));
00628
00629 TMP4_XOC =
00630             + VAT3( oPS, ii,jj,kk) * (- VAT3( oE, im1,jm1, k) * VAT3(oPSW, ii,jj,kk)
00631             - VAT3( uC, i, jm1,kml) * VAT3( dPS, ii,jj,kk)
00632             + VAT3( oC, i, jm1, k) * VAT3( oPS, ii,jj,kk)
00633             - VAT3( uC, i, jm1, k) * VAT3( uPS, ii,jj,kk)
00634             - VAT3( oN, i, jm1, k) * VAT3( oPC, ii,jj,kk)
00635             - VAT3( oE, i, jm1, k) * VAT3(oPSE, ii,jj,kk))
00636
00637             + VAT3( dPS, ii,jj,kk) * (- VAT3( oE, im1,jm1,kml) * VAT3(dPSW, ii,jj,kk)
00638             + VAT3( oC, i, jm1,kml) * VAT3( dPS, ii,jj,kk)
00639             - VAT3( uC, i, jm1,kml) * VAT3( oPS, ii,jj,kk)
00640             - VAT3( oN, i, jm1,kml) * VAT3( dPC, ii,jj,kk)
00641             - VAT3( oE, i, jm1,kml) * VAT3(dPSE, ii,jj,kk))
00642
00643             + VAT3(oPSE, ii,jj,kk) * (- VAT3( oE, i, jm1, k) * VAT3( oPS, ii,jj,kk)
00644             - VAT3( uC, ip1,jm1,kml) * VAT3(dPSE, ii,jj,kk)
00645             + VAT3( oC, ip1,jm1, k) * VAT3(oPSE, ii,jj,kk)
00646             - VAT3( uC, ip1,jm1, k) * VAT3(uPSE, ii,jj,kk)
00647             - VAT3( oN, ip1,jm1, k) * VAT3( oPE, ii,jj,kk));
00648
00649 TMP5_XOC =
00650             + VAT3( dPN, ii,jj,kk) * (- VAT3( oE, im1,jp1,kml) * VAT3(dPNW, ii,jj,kk)
00651             - VAT3( oN, i, j,kml) * VAT3( dPC, ii,jj,kk)
00652             + VAT3( oC, i, jp1,kml) * VAT3( dPN, ii,jj,kk)
00653             - VAT3( uC, i, jp1,kml) * VAT3( oPN, ii,jj,kk)
00654             - VAT3( oE, i, jp1,kml) * VAT3(dPNE, ii,jj,kk))
00655
00656             + VAT3( uPC, ii,jj,kk) * (- VAT3( oE, im1, j,kp1) * VAT3( uPW, ii,jj,kk)
00657             - VAT3( oN, i, jm1,kp1) * VAT3( uPS, ii,jj,kk)
00658             - VAT3( uC, i, j, k) * VAT3( oPC, ii,jj,kk)
00659             + VAT3( oC, i, j,kp1) * VAT3( uPC, ii,jj,kk)
00660             - VAT3( oN, i, j,kp1) * VAT3( uPN, ii,jj,kk)
00661             - VAT3( oE, i, j,kp1) * VAT3( uPE, ii,jj,kk))
00662
00663             + VAT3( oPC, ii,jj,kk) * (- VAT3( oE, im1, j, k) * VAT3( oPW, ii,jj,kk)
00664             - VAT3( oN, i, jm1, k) * VAT3( oPS, ii,jj,kk)
00665             - VAT3( uC, i, j,kml) * VAT3( dPC, ii,jj,kk)
00666             + VAT3( oC, i, j, k) * VAT3( oPC, ii,jj,kk)
00667             - VAT3( uC, i, j, k) * VAT3( uPC, ii,jj,kk)
00668             - VAT3( oN, i, j, k) * VAT3( oPN, ii,jj,kk)
00669             - VAT3( oE, i, j, k) * VAT3( oPE, ii,jj,kk));
00670
00671 TMP6_XOC =
00672             + VAT3( dPC, ii,jj,kk) * (- VAT3( oE, im1, j,kml) * VAT3( dPW, ii,jj,kk)
00673             - VAT3( oN, i, jm1,kml) * VAT3( dPS, ii,jj,kk)
00674             + VAT3( oC, i, j,kml) * VAT3( dPC, ii,jj,kk)
00675             - VAT3( uC, i, j,kml) * VAT3( oPC, ii,jj,kk)
00676             - VAT3( oN, i, j,kml) * VAT3( dPN, ii,jj,kk)
00677             - VAT3( oE, i, j,kml) * VAT3( dPE, ii,jj,kk))
00678
00679             + VAT3( uPS, ii,jj,kk) * (- VAT3( oE, im1,jm1,kp1) * VAT3(uPSW, ii,jj,kk)
00680             - VAT3( uC, i, jm1, k) * VAT3( oPS, ii,jj,kk)

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00681             + VAT3( oC, i,jm1,kp1) * VAT3( uPS, ii,jj,kk)
00682             - VAT3( oN, i,jm1,kp1) * VAT3( uPC, ii,jj,kk)
00683             - VAT3( oE, i,jm1,kp1) * VAT3(uPSE, ii,jj,kk))
00684
00685         + VAT3(uPNW, ii,jj,kk) * (- VAT3( oN, im1, j,kp1) * VAT3( uPW, ii,jj,kk)
00686             - VAT3( uC, im1,jp1, k) * VAT3(oPNW, ii,jj,kk)
00687             + VAT3( oC, im1,jp1,kp1) * VAT3(uPNW, ii,jj,kk)
00688             - VAT3( oE, im1,jp1,kp1) * VAT3( uPN, ii,jj,kk));
00689
00690     TMP7_XOC =
00691         + VAT3( dPW, ii,jj,kk) * (- VAT3( oN, im1,jm1,kml) * VAT3(dPSW, ii,jj,kk)
00692             + VAT3( oC, im1, j,kml) * VAT3( dPW, ii,jj,kk)
00693             - VAT3( uC, im1, j,kml) * VAT3( oPW, ii,jj,kk)
00694             - VAT3( oN, im1, j,kml) * VAT3(dPNW, ii,jj,kk)
00695             - VAT3( oE, im1, j,kml) * VAT3( dPC, ii,jj,kk))
00696
00697         + VAT3(uPSW, ii,jj,kk) * (- VAT3( uC, im1,jm1, k) * VAT3(oPSW, ii,jj,kk)
00698             + VAT3( oC, im1,jm1,kp1) * VAT3(uPSW, ii,jj,kk)
00699             - VAT3( oN, im1,jm1,kp1) * VAT3( uPW, ii,jj,kk)
00700             - VAT3( oE, im1,jm1,kp1) * VAT3( uPS, ii,jj,kk))
00701
00702         + VAT3(oPSW, ii,jj,kk) * (- VAT3( uC, im1,jm1,kml) * VAT3(dPSW, ii,jj,kk)
00703             + VAT3( oC, im1,jm1, k) * VAT3(oPSW, ii,jj,kk)
00704             + VAT3( uC, im1,jm1, k) * VAT3(uPSW, ii,jj,kk)
00705             - VAT3( oN, im1,jm1, k) * VAT3( oPW, ii,jj,kk)
00706             - VAT3( oE, im1,jm1, k) * VAT3( oPS, ii,jj,kk));
00707
00708     TMP8_XOC =
00709         + VAT3(oPNW, ii,jj,kk) * (- VAT3( oN, im1, j, k) * VAT3( oPW, ii,jj,kk)
00710             - VAT3( uC, im1,jp1,kml) * VAT3(dPNW, ii,jj,kk)
00711             + VAT3( oC, im1,jp1, k) * VAT3(oPNW, ii,jj,kk)
00712             - VAT3( uC, im1,jp1, k) * VAT3(uPNW, ii,jj,kk)
00713             - VAT3( oE, im1,jp1, k) * VAT3( oPN, ii,jj,kk))
00714
00715         + VAT3(dPNW, ii,jj,kk) * (- VAT3( oN, im1, j,kml) * VAT3( dPW, ii,jj,kk)
00716             + VAT3( oC, im1,jp1,kml) * VAT3(dPNW, ii,jj,kk)
00717             - VAT3( uC, im1,jp1,kml) * VAT3(oPNW, ii,jj,kk)
00718             - VAT3( oE, im1,jp1,kml) * VAT3( dPN, ii,jj,kk))
00719
00720         + VAT3( oPW, ii,jj,kk) * (- VAT3( oN, im1,jm1, k) * VAT3(oPSW, ii,jj,kk)
00721             - VAT3( uC, im1, j,kml) * VAT3( dPW, ii,jj,kk)
00722             + VAT3( oC, im1, j, k) * VAT3( oPW, ii,jj,kk)
00723             - VAT3( uC, im1, j, k) * VAT3( uPW, ii,jj,kk)
00724             - VAT3( oN, im1, j, k) * VAT3(oPNW, ii,jj,kk)
00725             - VAT3( oE, im1, j, k) * VAT3( oPC, ii,jj,kk));
00726
00727     TMP9_XOC =
00728         + VAT3( uPW, ii,jj,kk) * (- VAT3( oN, im1,jm1,kp1) * VAT3(uPSW, ii,jj,kk)
00729             - VAT3( uC, im1, j, k) * VAT3( oPW, ii,jj,kk)
00730             + VAT3( oC, im1, j,kp1) * VAT3( uPW, ii,jj,kk)
00731             - VAT3( oN, im1, j,kp1) * VAT3(uPNW, ii,jj,kk)
00732             - VAT3( oE, im1, j,kp1) * VAT3( uPC, ii,jj,kk))
00733
00734         + VAT3( uPN, ii,jj,kk) * (- VAT3( oE, im1,jp1,kp1) * VAT3(uPNW, ii,jj,kk)
00735             - VAT3( oN, i, j,kp1) * VAT3( uPC, ii,jj,kk)
00736             - VAT3( uC, i,jp1, k) * VAT3( oPN, ii,jj,kk)
00737             + VAT3( oC, i,jp1,kp1) * VAT3( uPN, ii,jj,kk)
00738             - VAT3( oE, i,jp1,kp1) * VAT3(uPNE, ii,jj,kk))
00739
00740         + VAT3( oPN, ii,jj,kk) * (- VAT3( oE, im1,jp1, k) * VAT3(oPNW, ii,jj,kk)
00741             - VAT3( oN, i, j, k) * VAT3( oPC, ii,jj,kk)
00742             - VAT3( uC, i,jp1,kml) * VAT3( dPN, ii,jj,kk)
00743             + VAT3( oC, i,jp1, k) * VAT3( oPN, ii,jj,kk)
00744             - VAT3( uC, i,jp1, k) * VAT3( uPN, ii,jj,kk)
00745             - VAT3( oE, i,jp1, k) * VAT3(oPNE, ii,jj,kk));
00746
00747     VAT3( XoC, ii,jj,kk) = TMP1_XOC + TMP2_XOC + TMP3_XOC
00748         + TMP4_XOC + TMP5_XOC + TMP6_XOC
00749         + TMP7_XOC + TMP8_XOC + TMP9_XOC;
00750
00751     //fprintf(data, "%19.12E\n", VAT3(XoC, ii, jj, kk));
00752
00753     /* *****
00754     * *** > oE;
00755     * *****
00756
00757     // VAT3( XoE, ii,jj,kk) =
00758     TMP1_XOE =
00759         VAT3( dPS, ii,jj,kk) * VAT3( oE, i,jm1,kml) * VAT3(dPSW, iip1,jj,kk)
00760         + VAT3( oPS, ii,jj,kk) * VAT3( oE, i,jm1, k) * VAT3(oPSW, iip1,jj,kk)
00761         + VAT3( uPS, ii,jj,kk) * VAT3( oE, i,jm1,kp1) * VAT3(uPSW, iip1,jj,kk)

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00762      + VAT3( dPC, ii,jj,kk) * VAT3( oE, i, j, kml) * VAT3( dPW, iip1,jj,kk)
00763      + VAT3( oPC, ii,jj,kk) * VAT3( oE, i, j, k) * VAT3( oPW, iip1,jj,kk)
00764      + VAT3( uPC, ii,jj,kk) * VAT3( oE, i, j, kpl) * VAT3( uPW, iip1,jj,kk)
00765      + VAT3( dPN, ii,jj,kk) * VAT3( oE, i, jpl, kml) * VAT3( dPNW, iip1,jj,kk)
00766      + VAT3( oPN, ii,jj,kk) * VAT3( oE, i, jpl, k) * VAT3( oPNW, iip1,jj,kk)
00767      + VAT3( uPN, ii,jj,kk) * VAT3( oE, i, jpl, kpl) * VAT3( uPNW, iip1,jj,kk)
00768
00769      - VAT3(dPSE, ii,jj,kk) * ( VAT3( oC, ip1,jml,kml) * VAT3(dPSW, iip1,jj,kk)
00770          - VAT3( uC, ip1,jml,kml) * VAT3(oPSW, iip1,jj,kk)
00771          - VAT3( oN, ip1,jml,kml) * VAT3( dPW, iip1,jj,kk)
00772          - VAT3( oE, ip1,jml,kml) * VAT3( dPS, iip1,jj,kk));
00773
00774      TMP2_XOE =
00775      - VAT3(oPSE, ii,jj,kk) * (- VAT3( uC, ip1,jml,kml) * VAT3(dPSW, iip1,jj,kk)
00776          + VAT3( oC, ip1,jml, k) * VAT3(oPSW, iip1,jj,kk)
00777          - VAT3( uC, ip1,jml, k) * VAT3(uPSW, iip1,jj,kk)
00778          - VAT3( oN, ip1,jml, k) * VAT3( oPW, iip1,jj,kk)
00779          - VAT3( oE, ip1,jml, k) * VAT3( oPS, iip1,jj,kk))
00780
00781      - VAT3(uPSE, ii,jj,kk) * (- VAT3( uC, ip1,jml, k) * VAT3(oPSW, iip1,jj,kk)
00782          + VAT3( oC, ip1,jml,kpl) * VAT3(uPSW, iip1,jj,kk)
00783          - VAT3( oN, ip1,jml,kpl) * VAT3( uPW, iip1,jj,kk)
00784          - VAT3( oE, ip1,jml,kpl) * VAT3( uPS, iip1,jj,kk))
00785
00786      - VAT3( dPE, ii,jj,kk) * (- VAT3( oN, ip1,jml,kml) * VAT3(dPSW, iip1,jj,kk)
00787          + VAT3( oC, ip1, j,kml) * VAT3( dPW, iip1,jj,kk)
00788          - VAT3( uC, ip1, j,kml) * VAT3( oPW, iip1,jj,kk)
00789          - VAT3( oN, ip1, j,kml) * VAT3(dPNW, iip1,jj,kk)
00790          - VAT3( oE, ip1, j,kml) * VAT3( dPC, iip1,jj,kk));
00791
00792      TMP3_XOE =
00793      - VAT3( oPE, ii,jj,kk) * (- VAT3( oN, ip1,jml, k) * VAT3(oPSW, iip1,jj,kk)
00794          - VAT3( uC, ip1, j,kml) * VAT3( dPW, iip1,jj,kk)
00795          + VAT3( oC, ip1, j, k) * VAT3( oPW, iip1,jj,kk)
00796          - VAT3( uC, ip1, j, k) * VAT3( uPW, iip1,jj,kk)
00797          - VAT3( oN, ip1, j, k) * VAT3(oPNW, iip1,jj,kk)
00798          - VAT3( oE, ip1, j, k) * VAT3( oPC, iip1,jj,kk))
00799
00800      - VAT3( uPE, ii,jj,kk) * (- VAT3( oN, ip1,jml,kpl) * VAT3(uPSW, iip1,jj,kk)
00801          - VAT3( uC, ip1, j, k) * VAT3( oPW, iip1,jj,kk)
00802          + VAT3( oC, ip1, j,kpl) * VAT3( uPW, iip1,jj,kk)
00803          - VAT3( oN, ip1, j,kpl) * VAT3(uPNW, iip1,jj,kk)
00804          - VAT3( oE, ip1, j,kpl) * VAT3( uPC, iip1,jj,kk))
00805
00806      - VAT3(dPNE, ii,jj,kk) * (- VAT3( oN, ip1, j,kml) * VAT3( dPW, iip1,jj,kk)
00807          + VAT3( oC, ip1,jpl,kml) * VAT3(dPNW, iip1,jj,kk)
00808          - VAT3( uC, ip1,jpl,kml) * VAT3(oPNW, iip1,jj,kk)
00809          - VAT3( oE, ip1,jpl,kml) * VAT3( dPN, iip1,jj,kk));
00810
00811      TMP4_XOE =
00812      - VAT3(oPNE, ii,jj,kk) * (- VAT3( oN, ip1, j, k) * VAT3( oPW, iip1,jj,kk)
00813          - VAT3( uC, ip1,jpl,kml) * VAT3(dPNW, iip1,jj,kk)
00814          + VAT3( oC, ip1,jpl, k) * VAT3(oPNW, iip1,jj,kk)
00815          - VAT3( uC, ip1,jpl, k) * VAT3(uPNW, iip1,jj,kk)
00816          - VAT3( oE, ip1,jpl, k) * VAT3( oPN, iip1,jj,kk))
00817
00818      - VAT3(uPNE, ii,jj,kk) * (- VAT3( oN, ip1, j,kpl) * VAT3( uPW, iip1,jj,kk)
00819          - VAT3( uC, ip1,jpl, k) * VAT3(oPNW, iip1,jj,kk)
00820          + VAT3( oC, ip1,jpl,kpl) * VAT3(uPNW, iip1,jj,kk)
00821          - VAT3( oE, ip1,jpl,kpl) * VAT3( uPN, iip1,jj,kk));
00822
00823      VAT3( XoE, ii,jj,kk) = TMP1_XOE + TMP2_XOE + TMP3_XOE + TMP4_XOE;
00824
00825      //fprintf(data, "%19.12E\n", VAT3(XoE, ii, jj, kk));
00826
00827
00828
00829      /* *****
00830      * *** > oN;
00831      * *****
00832
00833      // VAT3( XoN, ii,jj,kk) =
00834      TMP1_XON =
00835      VAT3( dPW, ii,jj,kk) * VAT3( oN, iml,j,kml) * VAT3(dPSW, ii,jjpl,kk)
00836      + VAT3( oPW, ii,jj,kk) * VAT3( oN, iml,j,k) * VAT3(oPSW, ii,jjpl,kk)
00837      + VAT3( uPW, ii,jj,kk) * VAT3( oN, iml,j,kpl) * VAT3(uPSW, ii,jjpl,kk)
00838
00839      - VAT3(dPNW, ii,jj,kk) * ( VAT3( oC, iml,jpl,kml) * VAT3(dPSW, ii,jjpl,kk)
00840          - VAT3( uC, iml,jpl,kml) * VAT3(oPSW, ii,jjpl,kk)
00841          - VAT3( oN, iml,jpl,kml) * VAT3( dPW, ii,jjpl,kk)
00842          - VAT3( oE, iml,jpl,kml) * VAT3( dPS, ii,jjpl,kk))
00843

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00844     - VAT3(oPNW, ii,jj,kk) * (- VAT3( uC, iml,jpl,kml) * VAT3(dPSW, ii,jjp1,kk)
00845       + VAT3( oC, iml,jpl,k) * VAT3(oPSW, ii,jjp1,kk)
00846       - VAT3( uC, iml,jpl,k) * VAT3(uPSW, ii,jjp1,kk)
00847       - VAT3( oN, iml,jpl,k) * VAT3( oPW, ii,jjp1,kk)
00848       - VAT3( oE, iml,jpl,k) * VAT3( oPS, ii,jjp1,kk));
00849
00850     TMP2_XON =
00851     - VAT3(uPNW, ii,jj,kk) * (- VAT3( uC, iml,jpl,k) * VAT3(oPSW, ii,jjp1,kk)
00852       + VAT3( oC, iml,jpl,kpl) * VAT3(uPSW, ii,jjp1,kk)
00853       - VAT3( oN, iml,jpl,kpl) * VAT3( uPW, ii,jjp1,kk)
00854       - VAT3( oE, iml,jpl,kpl) * VAT3( uPS, ii,jjp1,kk))
00855
00856     + VAT3( dPC, ii,jj,kk) * VAT3( oN, i,j,kml) * VAT3( dPS, ii,jjp1,kk)
00857     + VAT3( oPC, ii,jj,kk) * VAT3( oN, i,j,k) * VAT3( oPS, ii,jjp1,kk)
00858     + VAT3( uPC, ii,jj,kk) * VAT3( oN, i,j,kpl) * VAT3( uPS, ii,jjp1,kk)
00859
00860     - VAT3( dPN, ii,jj,kk) * (- VAT3( oE, iml,jpl,kml) * VAT3(dPSW, ii,jjp1,kk)
00861       + VAT3( oC, i,jpl,kml) * VAT3( dPS, ii,jjp1,kk)
00862       - VAT3( uC, i,jpl,kml) * VAT3( oPS, ii,jjp1,kk)
00863       - VAT3( oN, i,jpl,kml) * VAT3( dPC, ii,jjp1,kk)
00864       - VAT3( oE, i,jpl,kml) * VAT3(dPSE, ii,jjp1,kk));
00865
00866     TMP3_XON =
00867     - VAT3( oPN, ii,jj,kk) * (- VAT3( oE, iml,jpl,k) * VAT3(oPSW, ii,jjp1,kk)
00868       - VAT3( uC, i,jpl,kml) * VAT3( dPS, ii,jjp1,kk)
00869       + VAT3( oC, i,jpl,k) * VAT3( oPS, ii,jjp1,kk)
00870       - VAT3( uC, i,jpl,k) * VAT3( uPS, ii,jjp1,kk)
00871       - VAT3( oN, i,jpl,k) * VAT3( oPC, ii,jjp1,kk)
00872       - VAT3( oE, i,jpl,k) * VAT3(oPSE, ii,jjp1,kk))
00873
00874     - VAT3( uPN, ii,jj,kk) * (- VAT3( oE, iml,jpl,kpl) * VAT3(uPSW, ii,jjp1,kk)
00875       - VAT3( uC, i,jpl,k) * VAT3( oPS, ii,jjp1,kk)
00876       + VAT3( oC, i,jpl,kpl) * VAT3( uPS, ii,jjp1,kk)
00877       - VAT3( oN, i,jpl,kpl) * VAT3( uPC, ii,jjp1,kk)
00878       - VAT3( oE, i,jpl,kpl) * VAT3(uPSE, ii,jjp1,kk))
00879
00880     + VAT3( dPE, ii,jj,kk) * VAT3( oN, ipl,j,kml) * VAT3(dPSE, ii,jjp1,kk)
00881     + VAT3( oPE, ii,jj,kk) * VAT3( oN, ipl,j,k) * VAT3(oPSE, ii,jjp1,kk)
00882     + VAT3( uPE, ii,jj,kk) * VAT3( oN, ipl,j,kpl) * VAT3(uPSE, ii,jjp1,kk);
00883
00884     TMP4_XON =
00885     - VAT3(dPNE, ii,jj,kk) * (- VAT3( oE, i,jpl,kml) * VAT3( dPS, ii,jjp1,kk)
00886       + VAT3( oC, ipl,jpl,kml) * VAT3(dPSE, ii,jjp1,kk)
00887       - VAT3( uC, ipl,jpl,kml) * VAT3(oPSE, ii,jjp1,kk)
00888       - VAT3( oN, ipl,jpl,kml) * VAT3( dPE, ii,jjp1,kk))
00889
00890     - VAT3(oPNE, ii,jj,kk) * (- VAT3( oE, i,jpl,k) * VAT3( oPS, ii,jjp1,kk)
00891       - VAT3( uC, ipl,jpl,kml) * VAT3(dPSE, ii,jjp1,kk)
00892       + VAT3( oC, ipl,jpl,k) * VAT3(oPSE, ii,jjp1,kk)
00893       - VAT3( uC, ipl,jpl,k) * VAT3(uPSE, ii,jjp1,kk)
00894       - VAT3( oN, ipl,jpl,k) * VAT3( oPE, ii,jjp1,kk))
00895
00896     - VAT3(uPNE, ii,jj,kk) * (- VAT3( oE, i,jpl,kpl) * VAT3( uPS, ii,jjp1,kk)
00897       - VAT3( uC, ipl,jpl,k) * VAT3(oPSE, ii,jjp1,kk)
00898       + VAT3( oC, ipl,jpl,kpl) * VAT3(uPSE, ii,jjp1,kk)
00899       - VAT3( oN, ipl,jpl,kpl) * VAT3( uPE, ii,jjp1,kk));
00900
00901     VAT3( XoN, ii,jj,kk) = TMP1_XON + TMP2_XON + TMP3_XON + TMP4_XON;
00902
00903     //fprintf(data, "%19.12E\n", VAT3(XoN, ii, jj, kk));
00904
00905     /* *****
00906     * *** > uC;
00907     * *****
00908
00909     // VAT3( XuC, ii,jj,kk) =
00910     TMP1_XUC =
00911     VAT3(oPSW, ii,jj,kk) * VAT3( uC, iml,jml,k) * VAT3(dPSW, ii,jj,kkpl)
00912
00913     - VAT3(uPSW, ii,jj,kk) * ( VAT3( oC, iml,jml,kpl) * VAT3(dPSW, ii,jj,kkpl)
00914       - VAT3( uC, iml,jml,kpl) * VAT3(oPSW, ii,jj,kkpl)
00915       - VAT3( oN, iml,jml,kpl) * VAT3( dPW, ii,jj,kkpl)
00916       - VAT3( oE, iml,jml,kpl) * VAT3( dPS, ii,jj,kkpl))
00917
00918     + VAT3( oPW, ii,jj,kk) * VAT3( uC, iml,j,k) * VAT3( dPW, ii,jj,kkpl)
00919
00920     - VAT3( uPW, ii,jj,kk) * (- VAT3( oN, iml,jml,kpl) * VAT3(dPSW, ii,jj,kkpl)
00921       + VAT3( oC, iml,j,kpl) * VAT3( dPW, ii,jj,kkpl)
00922       - VAT3( uC, iml,j,kpl) * VAT3( oPW, ii,jj,kkpl)
00923       - VAT3( oN, iml,j,kpl) * VAT3(dPNW, ii,jj,kkpl)
00924       - VAT3( oE, iml,j,kpl) * VAT3( dPC, ii,jj,kkpl))

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00925
00926      + VAT3(oPNW, ii,jj,kk) * VAT3( uC, im1,jp1,k) * VAT3(dPNW, ii,jj,kkp1);
00927
00928  TMP2_XUC =
00929      - VAT3(uPNW, ii,jj,kk) * (- VAT3( oN, im1,j,kp1) * VAT3( dPW, ii,jj,kkp1)
00930        + VAT3( oC, im1,jp1,kp1) * VAT3(dPNW, ii,jj,kkp1)
00931        - VAT3( uC, im1,jp1,kp1) * VAT3(oPNW, ii,jj,kkp1)
00932        - VAT3( oE, im1,jp1,kp1) * VAT3( dPN, ii,jj,kkp1))
00933
00934      + VAT3( oPS, ii,jj,kk) * VAT3( uC, i,jm1,k) * VAT3( dPS, ii,jj,kkp1)
00935
00936      - VAT3( uPS, ii,jj,kk) * (- VAT3( oE, im1,jm1,kp1) * VAT3(dPSW, ii,jj,kkp1)
00937        + VAT3( oC, i,jm1,kp1) * VAT3( dPS, ii,jj,kkp1)
00938        - VAT3( uC, i,jm1,kp1) * VAT3( oPS, ii,jj,kkp1)
00939        - VAT3( oN, i,jm1,kp1) * VAT3( dPC, ii,jj,kkp1)
00940        - VAT3( oE, i,jm1,kp1) * VAT3(dPSE, ii,jj,kkp1))
00941
00942      + VAT3( oPC, ii,jj,kk) * VAT3( uC, i,j,k) * VAT3( dPC, ii,jj,kkp1)
00943
00944      - VAT3( uPC, ii,jj,kk) * (- VAT3( oE, im1,j,kp1) * VAT3( dPW, ii,jj,kkp1)
00945        - VAT3( oN, i,jm1,kp1) * VAT3( dPS, ii,jj,kkp1)
00946        + VAT3( oC, i,j,kp1) * VAT3( dPC, ii,jj,kkp1)
00947        - VAT3( uC, i,j,kp1) * VAT3( oPC, ii,jj,kkp1)
00948        - VAT3( oN, i,j,kp1) * VAT3( dPN, ii,jj,kkp1)
00949        - VAT3( oE, i,j,kp1) * VAT3( dPE, ii,jj,kkp1));
00950
00951  TMP3_XUC =
00952      + VAT3( oPN, ii,jj,kk) * VAT3( uC, i,jp1,k) * VAT3( dPN, ii,jj,kkp1)
00953
00954      - VAT3( uPN, ii,jj,kk) * (- VAT3( oE, im1,jp1,kp1) * VAT3(dPNW, ii,jj,kkp1)
00955        - VAT3( oN, i,j,kp1) * VAT3( dPC, ii,jj,kkp1)
00956        + VAT3( oC, i,jp1,kp1) * VAT3( dPN, ii,jj,kkp1)
00957        - VAT3( uC, i,jp1,kp1) * VAT3( oPN, ii,jj,kkp1)
00958        - VAT3( oE, i,jp1,kp1) * VAT3(dPNE, ii,jj,kkp1))
00959
00960      + VAT3(oPSE, ii,jj,kk) * VAT3( uC, ip1,jm1,k) * VAT3(dPSE, ii,jj,kkp1)
00961
00962      - VAT3(uPSE, ii,jj,kk) * (- VAT3( oE, i,jm1,kp1) * VAT3( dPS, ii,jj,kkp1)
00963        + VAT3( oC, ip1,jm1,kp1) * VAT3(dPSE, ii,jj,kkp1)
00964        - VAT3( uC, ip1,jm1,kp1) * VAT3(oPSE, ii,jj,kkp1)
00965        - VAT3( oN, ip1,jm1,kp1) * VAT3( dPE, ii,jj,kkp1));
00966
00967  TMP4_XUC =
00968      + VAT3( oPE, ii,jj,kk) * VAT3( uC, ip1,j,k) * VAT3( dPE, ii,jj,kkp1)
00969
00970      - VAT3( uPE, ii,jj,kk) * (- VAT3( oE, i,j,kp1) * VAT3( dPC, ii,jj,kkp1)
00971        - VAT3( oN, ip1,jm1,kp1) * VAT3(dPSE, ii,jj,kkp1)
00972        + VAT3( oC, ip1,j,kp1) * VAT3( dPE, ii,jj,kkp1)
00973        - VAT3( uC, ip1,j,kp1) * VAT3( oPE, ii,jj,kkp1)
00974        - VAT3( oN, ip1,j,kp1) * VAT3(dPNE, ii,jj,kkp1))
00975
00976      + VAT3(oPNE, ii,jj,kk) * VAT3( uC, ip1,jp1,k) * VAT3(dPNE, ii,jj,kkp1)
00977
00978      - VAT3(uPNE, ii,jj,kk) * (- VAT3( oE, i,jp1,kp1) * VAT3( dPN, ii,jj,kkp1)
00979        - VAT3( oN, ip1,j,kp1) * VAT3( dPE, ii,jj,kkp1)
00980        + VAT3( oC, ip1,jp1,kp1) * VAT3(dPNE, ii,jj,kkp1)
00981        - VAT3( uC, ip1,jp1,kp1) * VAT3(oPNE, ii,jj,kkp1));
00982
00983  VAT3( XuC, ii,jj,kk) = TMP1_XUC + TMP2_XUC + TMP3_XUC + TMP4_XUC;
00984
00985      //fprintf(data, "%19.12E\n", VAT3(XuC, ii, jj, kk));
00986
00987      /* *****
00988      * *** > oNE;
00989      * *****/
00990
00991  VAT3( XoNE, ii,jj,kk) =
00992      VAT3( dPN, ii,jj,kk) * VAT3( oE, i,jp1,kml) * VAT3(dPSW, iip1,jjp1,kk)
00993      + VAT3( oPN, ii,jj,kk) * VAT3( oE, i,jp1,k) * VAT3(oPSW, iip1,jjp1,kk)
00994      + VAT3( uPN, ii,jj,kk) * VAT3( oE, i,jp1,kp1) * VAT3(uPSW, iip1,jjp1,kk)
00995      + VAT3( dPE, ii,jj,kk) * VAT3( oN, ip1,j,kml) * VAT3(dPSW, iip1,jjp1,kk)
00996      + VAT3( oPE, ii,jj,kk) * VAT3( oN, ip1,j,k) * VAT3(oPSW, iip1,jjp1,kk)
00997      + VAT3( uPE, ii,jj,kk) * VAT3( oN, ip1,j,kp1) * VAT3(uPSW, iip1,jjp1,kk)
00998
00999      - VAT3(dPNE, ii,jj,kk) * ( VAT3( oC, ip1,jp1,kml) * VAT3(dPSW, iip1,jjp1,kk)
01000        - VAT3( uC, ip1,jp1,kml) * VAT3(oPSW, iip1,jjp1,kk)
01001        - VAT3( oN, ip1,jp1,kml) * VAT3( dPW, iip1,jjp1,kk)
01002        - VAT3( oE, ip1,jp1,kml) * VAT3( dPS, iip1,jjp1,kk))
01003
01004      - VAT3(oPNE, ii,jj,kk) * (- VAT3( uC, ip1,jp1,kml) * VAT3(dPSW, iip1,jjp1,kk)
01005        + VAT3( oC, ip1,jp1,k) * VAT3(oPSW, iip1,jjp1,kk)

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01006             - VAT3( uC, ip1,jp1,k) * VAT3(uPSW, iip1,jjp1,kk)
01007             - VAT3( oN, ip1,jp1,k) * VAT3( oPW, iip1,jjp1,kk)
01008             - VAT3( oE, ip1,jp1,k) * VAT3( oPS, iip1,jjp1,kk))
01009
01010         - VAT3(uPNE, ii,jj,kk) * (- VAT3( uC, ip1,jp1,k) * VAT3(oPSW, iip1,jjp1,kk)
01011           + VAT3( oC, ip1,jp1,kp1) * VAT3(uPSW, iip1,jjp1,kk)
01012           - VAT3( oN, ip1,jp1,kp1) * VAT3( uPW, iip1,jjp1,kk)
01013           - VAT3( oE, ip1,jp1,kp1) * VAT3( uPS, iip1,jjp1,kk));
01014
01015         //fprintf(data, "%19.12E\n", VAT3(XoNE, ii, jj, kk));
01016
01017         /* *****
01018          * *** > oNW;
01019          * *****/
01020
01021         VAT3(XoNW, ii,jj,kk) =
01022             VAT3( dPW, ii,jj,kk) * VAT3( oN, im1,j,kml) * VAT3(dPSE, iim1,jjp1,kk)
01023         + VAT3( oPW, ii,jj,kk) * VAT3( oN, im1,j,k) * VAT3(oPSE, iim1,jjp1,kk)
01024         + VAT3( uPW, ii,jj,kk) * VAT3( oN, im1,j,kp1) * VAT3(uPSE, iim1,jjp1,kk)
01025
01026         - VAT3(dPNW, ii,jj,kk) * (- VAT3( oE, im2,jp1,kml) * VAT3( dPS, iim1,jjp1,kk)
01027           + VAT3( oC, im1,jp1,kml) * VAT3(dPSE, iim1,jjp1,kk)
01028           - VAT3( uC, im1,jp1,kml) * VAT3(oPSE, iim1,jjp1,kk)
01029           - VAT3( oN, im1,jp1,kml) * VAT3( dPE, iim1,jjp1,kk))
01030
01031         - VAT3(oPNW, ii,jj,kk) * (- VAT3( oE, im2,jp1,k) * VAT3( oPS, iim1,jjp1,kk)
01032           - VAT3( uC, im1,jp1,kml) * VAT3(dPSE, iim1,jjp1,kk)
01033           + VAT3( oC, im1,jp1,k) * VAT3(oPSE, iim1,jjp1,kk)
01034           - VAT3( uC, im1,jp1,k) * VAT3(uPSE, iim1,jjp1,kk)
01035           - VAT3( oN, im1,jp1,k) * VAT3( oPE, iim1,jjp1,kk))
01036
01037         - VAT3(uPNW, ii,jj,kk) * (- VAT3( oE, im2,jp1,kp1) * VAT3( uPS, iim1,jjp1,kk)
01038           - VAT3( uC, im1,jp1,k) * VAT3(oPSE, iim1,jjp1,kk)
01039           + VAT3( oC, im1,jp1,kp1) * VAT3(uPSE, iim1,jjp1,kk)
01040           - VAT3( oN, im1,jp1,kp1) * VAT3( uPE, iim1,jjp1,kk))
01041
01042         + VAT3( dPN, ii,jj,kk) * VAT3( oE, im1,jp1,kml) * VAT3(dPSE, iim1,jjp1,kk)
01043         + VAT3( oPN, ii,jj,kk) * VAT3( oE, im1,jp1,k) * VAT3(oPSE, iim1,jjp1,kk)
01044         + VAT3( uPN, ii,jj,kk) * VAT3( oE, im1,jp1,kp1) * VAT3(uPSE, iim1,jjp1,kk);
01045
01046         //fprintf(data, "%19.12E\n", VAT3(XoNW, ii, jj, kk));
01047
01048         /* *****
01049          * *** > uE;
01050          * *****/
01051
01052         VAT3( XuE, ii,jj,kk) =
01053             VAT3( uPS, ii,jj,kk) * VAT3( oE, i,jml,kp1) * VAT3(dPSW, iip1,jj,kkp1)
01054         + VAT3( uPC, ii,jj,kk) * VAT3( oE, i,j,kp1) * VAT3( dPW, iip1,jj,kkp1)
01055         + VAT3( uPN, ii,jj,kk) * VAT3( oE, i,jp1,kp1) * VAT3(dPNW, iip1,jj,kkp1)
01056         + VAT3(oPSE, ii,jj,kk) * VAT3( uC, ip1,jml,k) * VAT3(dPSW, iip1,jj,kkp1)
01057
01058         - VAT3(uPSE, ii,jj,kk) * ( VAT3( oC, ip1,jml,kp1) * VAT3(dPSW, iip1,jj,kkp1)
01059           - VAT3( uC, ip1,jml,kp1) * VAT3(oPSW, iip1,jj,kkp1)
01060           - VAT3( oN, ip1,jml,kp1) * VAT3( dPW, iip1,jj,kkp1)
01061           - VAT3( oE, ip1,jml,kp1) * VAT3( dPS, iip1,jj,kkp1))
01062
01063         + VAT3( oPE, ii,jj,kk) * VAT3( uC, ip1,j,k) * VAT3( dPW, iip1,jj,kkp1)
01064
01065         - VAT3( uPE, ii,jj,kk) * (- VAT3( oN, ip1,jml,kp1) * VAT3(dPSW, iip1,jj,kkp1)
01066           + VAT3( oC, ip1,j,kp1) * VAT3( dPW, iip1,jj,kkp1)
01067           - VAT3( uC, ip1,j,kp1) * VAT3( oPW, iip1,jj,kkp1)
01068           - VAT3( oN, ip1,j,kp1) * VAT3(dPNW, iip1,jj,kkp1)
01069           - VAT3( oE, ip1,j,kp1) * VAT3( dPC, iip1,jj,kkp1))
01070
01071         + VAT3(oPNE, ii,jj,kk) * VAT3( uC, ip1,jp1,k) * VAT3(dPNW, iip1,jj,kkp1)
01072
01073         - VAT3(uPNE, ii,jj,kk) * (- VAT3( oN, ip1,j,kp1) * VAT3( dPW, iip1,jj,kkp1)
01074           + VAT3( oC, ip1,jp1,kp1) * VAT3(dPNW, iip1,jj,kkp1)
01075           - VAT3( uC, ip1,jp1,kp1) * VAT3(oPNW, iip1,jj,kkp1)
01076           - VAT3( oE, ip1,jp1,kp1) * VAT3( dPN, iip1,jj,kkp1));
01077
01078         //fprintf(data, "%19.12E\n", VAT3(XuE, ii, jj, kk));
01079
01080         /* *****
01081          * *** > uW;
01082          * *****/
01083
01084         VAT3( XuW, ii,jj,kk) =
01085             VAT3(oPSW, ii,jj,kk) * VAT3( uC, im1,jml,k) * VAT3(dPSE, iim1,jj,kkp1)
01086

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01087 - VAT3(uPSW, ii,jj,kk) * (- VAT3( oE, im2,jml,kp1) * VAT3( dPS, iim1,jj,kkp1)
01088 + VAT3( oC, im1,jml,kp1) * VAT3(dPSE, iim1,jj,kkp1)
01089 - VAT3( uC, im1,jml,kp1) * VAT3(oPSE, iim1,jj,kkp1)
01090 - VAT3( oN, im1,jml,kp1) * VAT3( dPE, iim1,jj,kkp1))
01091
01092 + VAT3( oPW, ii,jj,kk) * VAT3( uC, im1,j,k) * VAT3( dPE, iim1,jj,kkp1)
01093
01094 - VAT3( uPW, ii,jj,kk) * (- VAT3( oE, im2,j,kp1) * VAT3( dPC, iim1,jj,kkp1)
01095 - VAT3( oN, im1,jml,kp1) * VAT3(dPSE, iim1,jj,kkp1)
01096 + VAT3( oC, im1,j,kp1) * VAT3( dPE, iim1,jj,kkp1)
01097 - VAT3( uC, im1,j,kp1) * VAT3( oPE, iim1,jj,kkp1)
01098 - VAT3( oN, im1,j,kp1) * VAT3(dPNE, iim1,jj,kkp1))
01099
01100 + VAT3(oPNW, ii,jj,kk) * VAT3( uC, im1,jp1,k) * VAT3(dPNE, iim1,jj,kkp1)
01101
01102 - VAT3(uPNW, ii,jj,kk) * (- VAT3( oE, im2,jp1,kp1) * VAT3( dPN, iim1,jj,kkp1)
01103 - VAT3( oN, im1,j,kp1) * VAT3( dPE, iim1,jj,kkp1)
01104 + VAT3( oC, im1,jp1,kp1) * VAT3(dPNE, iim1,jj,kkp1)
01105 - VAT3( uC, im1,jp1,kp1) * VAT3(oPNE, iim1,jj,kkp1))
01106
01107 + VAT3( uPS, ii,jj,kk) * VAT3( oE, im1,jml,kp1) * VAT3(dPSE, iim1,jj,kkp1)
01108 + VAT3( uPC, ii,jj,kk) * VAT3( oE, im1,j,kp1) * VAT3( dPE, iim1,jj,kkp1)
01109 + VAT3( uPN, ii,jj,kk) * VAT3( oE, im1,jp1,kp1) * VAT3(dPNE, iim1,jj,kkp1);
01110
01111 //fprintf(data, "%19.12E\n", VAT3(XuW, ii, jj, kk));
01112
01113 /* *****
01114 * *** > uN;
01115 * *****/
01116
01117 VAT3( XuN, ii,jj,kk) =
01118 VAT3( uPW, ii,jj,kk) * VAT3( oN, im1,j,kp1) * VAT3(dPSW, ii,jjp1,kkp1)
01119 + VAT3(oPNW, ii,jj,kk) * VAT3( uC, im1,jp1,k) * VAT3(dPSW, ii,jjp1,kkp1)
01120
01121 - VAT3(uPNW, ii,jj,kk) * ( VAT3( oC, im1,jp1,kp1) * VAT3(dPSW, ii,jjp1,kkp1)
01122 - VAT3( uC, im1,jp1,kp1) * VAT3(oPSW, ii,jjp1,kkp1)
01123 - VAT3( oN, im1,jp1,kp1) * VAT3( dPW, ii,jjp1,kkp1)
01124 - VAT3( oE, im1,jp1,kp1) * VAT3( dPS, ii,jjp1,kkp1))
01125
01126 + VAT3( uPC, ii,jj,kk) * VAT3( oN, i,j,kp1) * VAT3( dPS, ii,jjp1,kkp1)
01127 + VAT3( oPN, ii,jj,kk) * VAT3( uC, i,jp1,k) * VAT3( dPS, ii,jjp1,kkp1)
01128
01129 - VAT3( uPN, ii,jj,kk) * (- VAT3( oE, im1,jp1,kp1) * VAT3(dPSW, ii,jjp1,kkp1)
01130 + VAT3( oC, i,jp1,kp1) * VAT3( dPS, ii,jjp1,kkp1)
01131 - VAT3( uC, i,jp1,kp1) * VAT3( oPS, ii,jjp1,kkp1)
01132 - VAT3( oN, i,jp1,kp1) * VAT3( dPC, ii,jjp1,kkp1)
01133 - VAT3( oE, i,jp1,kp1) * VAT3(dPSE, ii,jjp1,kkp1))
01134
01135 + VAT3( uPE, ii,jj,kk) * VAT3( oN, ip1,j,kp1) * VAT3(dPSE, ii,jjp1,kkp1)
01136 + VAT3(oPNE, ii,jj,kk) * VAT3( uC, ip1,jp1,k) * VAT3(dPSE, ii,jjp1,kkp1)
01137
01138 - VAT3(uPNE, ii,jj,kk) * (- VAT3( oE, i,jp1,kp1) * VAT3( dPS, ii,jjp1,kkp1)
01139 + VAT3( oC, ip1,jp1,kp1) * VAT3(dPSE, ii,jjp1,kkp1)
01140 - VAT3( uC, ip1,jp1,kp1) * VAT3(oPSE, ii,jjp1,kkp1)
01141 - VAT3( oN, ip1,jp1,kp1) * VAT3( dPE, ii,jjp1,kkp1));
01142
01143 //fprintf(data, "%19.12E\n", VAT3(XuN, ii, jj, kk));
01144
01145 /* *****
01146 * *** > uS;
01147 * *****/
01148
01149 VAT3( XuS, ii,jj,kk) =
01150 VAT3(oPSW, ii,jj,kk) * VAT3( uC, im1,jml,k) * VAT3(dPNW, ii,jjml,kkp1)
01151
01152 - VAT3(uPSW, ii,jj,kk) * (- VAT3( oN, im1,jm2,kp1) * VAT3( dPW, ii,jjml,kkp1)
01153 + VAT3( oC, im1,jml,kp1) * VAT3(dPNW, ii,jjml,kkp1)
01154 - VAT3( uC, im1,jml,kp1) * VAT3(oPNW, ii,jjml,kkp1)
01155 - VAT3( oE, im1,jml,kp1) * VAT3( dPN, ii,jjml,kkp1))
01156
01157 + VAT3( uPW, ii,jj,kk) * VAT3( oN, im1,jml,kp1) * VAT3(dPNW, ii,jjml,kkp1)
01158 + VAT3( oPS, ii,jj,kk) * VAT3( uC, i,jml,k) * VAT3( dPN, ii,jjml,kkp1)
01159
01160 - VAT3( uPS, ii,jj,kk) * (- VAT3( oE, im1,jml,kp1) * VAT3(dPNW, ii,jjml,kkp1)
01161 - VAT3( oN, i,jm2,kp1) * VAT3( dPC, ii,jjml,kkp1)
01162 + VAT3( oC, i,jml,kp1) * VAT3( dPN, ii,jjml,kkp1)
01163 - VAT3( uC, i,jml,kp1) * VAT3( oPN, ii,jjml,kkp1)
01164 - VAT3( oE, i,jml,kp1) * VAT3(dPNE, ii,jjml,kkp1))
01165
01166 + VAT3( uPC, ii,jj,kk) * VAT3( oN, i,jml,kp1) * VAT3( dPN, ii,jjml,kkp1)
01167 + VAT3(oPSE, ii,jj,kk) * VAT3( uC, ip1,jml,k) * VAT3(dPNE, ii,jjml,kkp1)

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01168
01169 - VAT3(uPSE, ii,jj,kk) * (- VAT3( oE, i,jm1,kp1) * VAT3( dPN, ii,jjm1,kkp1)
01170 - VAT3( oN, ip1,jm2,kp1) * VAT3( dPE, ii,jjm1,kkp1)
01171 + VAT3( oC, ip1,jm1,kp1) * VAT3( dPNE, ii,jjm1,kkp1)
01172 - VAT3( uC, ip1,jm1,kp1) * VAT3( oPNE, ii,jjm1,kkp1))
01173
01174 + VAT3( uPE, ii,jj,kk) * VAT3( oN, ip1,jm1,kp1) * VAT3( dPNE, ii,jjm1,kkp1);
01175
01176 //fprintf(data, "%19.12E\n", VAT3(XuS, ii, jj, kk));
01177
01178 /* *****
01179 * *** > uNE;
01180 * *****/
01181
01182 VAT3(XuNE, ii,jj,kk) =
01183 VAT3( uPN, ii,jj,kk) * VAT3( oE, i,jp1,kp1) * VAT3( dPSW, iip1,jjp1,kkp1)
01184 + VAT3( uPE, ii,jj,kk) * VAT3( oN, ip1,j,kp1) * VAT3( dPSW, iip1,jjp1,kkp1)
01185 + VAT3( oPNE, ii,jj,kk) * VAT3( uC, ip1,jp1,k) * VAT3( dPSW, iip1,jjp1,kkp1)
01186
01187 - VAT3( uPNE, ii,jj,kk) * ( VAT3( oC, ip1,jp1,kp1) * VAT3( dPSW, iip1,jjp1,kkp1)
01188 - VAT3( uC, im1,jp1,kp1) * VAT3( oPSW, iip1,jjp1,kkp1)
01189 - VAT3( oN, ip1,jp1,kp1) * VAT3( dPW, iip1,jjp1,kkp1)
01190 - VAT3( oE, ip1,jp1,kp1) * VAT3( dPS, iip1,jjp1,kkp1));
01191
01192 //fprintf(data, "%19.12E\n", VAT3(XuNE, ii, jj, kk));
01193
01194 /* *****
01195 * *** > uNW;
01196 * *****/
01197
01198 VAT3(XuNW, ii,jj,kk) =
01199 VAT3( uPW, ii,jj,kk) * VAT3( oN, im1,j,kp1) * VAT3( dPSE, iim1,jjp1,kkp1)
01200 + VAT3( oPNW, ii,jj,kk) * VAT3( uC, im1,jp1,k) * VAT3( dPSE, iim1,jjp1,kkp1)
01201
01202 - VAT3( uPNW, ii,jj,kk) * (- VAT3( oE, im2,jp1,kp1) * VAT3( dPS, iim1,jjp1,kkp1)
01203 + VAT3( oC, im1,jp1,kp1) * VAT3( dPSE, iim1,jjp1,kkp1)
01204 - VAT3( uC, im1,jp1,kp1) * VAT3( oPSE, iim1,jjp1,kkp1)
01205 - VAT3( oN, im1,jp1,kp1) * VAT3( dPE, iim1,jjp1,kkp1))
01206
01207 + VAT3( uPN, ii,jj,kk) * VAT3( oE, im1,jp1,kp1) * VAT3( dPSE, iim1,jjp1,kkp1);
01208
01209 //fprintf(data, "%19.12E\n", VAT3(XuNW, ii, jj, kk));
01210
01211 /* *****
01212 * *** > uSE;
01213 * *****/
01214
01215 VAT3(XuSE, ii,jj,kk) =
01216 VAT3( uPS, ii,jj,kk) * VAT3( oE, i,jm1,kp1) * VAT3( dPNW, iip1,jjm1,kkp1)
01217 + VAT3( oPSE, ii,jj,kk) * VAT3( uC, ip1,jm1,k) * VAT3( dPNW, iip1,jjm1,kkp1)
01218
01219 - VAT3( uPSE, ii,jj,kk) * (- VAT3( oN, ip1,jm2,kp1) * VAT3( dPW, iip1,jjm1,kkp1)
01220 + VAT3( oC, ip1,jm1,kp1) * VAT3( dPNW, iip1,jjm1,kkp1)
01221 - VAT3( uC, ip1,jm1,kp1) * VAT3( oPNW, iip1,jjm1,kkp1)
01222 - VAT3( oE, ip1,jm1,kp1) * VAT3( dPN, iip1,jjm1,kkp1))
01223
01224 + VAT3( uPE, ii,jj,kk) * VAT3( oN, ip1,jm1,kp1) * VAT3( dPNW, iip1,jjm1,kkp1);
01225
01226 //fprintf(data, "%19.12E\n", VAT3(XuSE, ii, jj, kk));
01227
01228 /* *****
01229 * *** > uSW;
01230 * *****/
01231
01232 VAT3(XuSW, ii,jj,kk) =
01233 VAT3( oPSW, ii,jj,kk) * VAT3( uC, im1,jm1,k) * VAT3( dPNE, iim1,jjm1,kkp1)
01234
01235 - VAT3( uPSW, ii,jj,kk) * (- VAT3( oE, im2,jm1,kp1) * VAT3( dPN, iim1,jjm1,kkp1)
01236 - VAT3( oN, im1,jm2,kp1) * VAT3( dPE, iim1,jjm1,kkp1)
01237 + VAT3( oC, im1,jm1,kp1) * VAT3( dPNE, iim1,jjm1,kkp1)
01238 - VAT3( uC, im1,jm1,kp1) * VAT3( oPNE, iim1,jjm1,kkp1))
01239
01240 + VAT3( uPW, ii,jj,kk) * VAT3( oN, im1,jm1,kp1) * VAT3( dPNE, iim1,jjm1,kkp1)
01241 + VAT3( uPS, ii,jj,kk) * VAT3( oE, im1,jm1,kp1) * VAT3( dPNE, iim1,jjm1,kkp1);
01242
01243 //fprintf(data, "%19.12E\n", VAT3(XuSW, ii, jj, kk));
01244
01245 }
01246 }
01247 }
01248 }

```

```

01249
01250
01251
01252 VPUBLIC void VbuildG_27(int *nxf, int *nyf, int *nzf,
01253     int *nx, int *ny, int *nz,
01254     double *oPC, double *oPN, double *oPS, double *oPE, double *oPW,
01255     double *oPNE, double *oPNW, double *oPSE, double *oPSW,
01256     double *uPC, double *uPN, double *uPS, double *uPE, double *uPW,
01257     double *uPNE, double *uPNW, double *uPSE, double *uPSW,
01258     double *dPC, double *dPN, double *dPS, double *dPE, double *dPW,
01259     double *dPNE, double *dPNW, double *dPSE, double *dPSW,
01260     double *oC, double *oE, double *oN, double *uC,
01261     double *oNE, double *oNW, double *uE, double *uW, double *uN,
01262     double *uS, double *uNE, double *uNW, double *uSE, double *uSW,
01263     double *XoC, double *XoE, double *XoN,
01264     double *XuC,
01265     double *XoNE, double *XoNW,
01266     double *XuE, double *XuW, double *XuN, double *XuS,
01267     double *XuNE, double *XuNW, double *XuSE, double *XuSW) {
01268
01269     int i, j, k;
01270     int ii, jj, kk;
01271     int im1, ip1, im2, ip2;
01272     int jm1, jp1, jm2, jp2;
01273     int km1, kp1, km2, kp2;
01274     int iim1, iip1;
01275     int jjm1, jjp1;
01276     int kkm1, kkp1;
01277     int nxm1, nym1, nzm1;
01278
01279     double TMP1_XOC, TMP2_XOC, TMP3_XOC, TMP4_XOC;
01280     double TMP5_XOC, TMP6_XOC, TMP7_XOC, TMP8_XOC;
01281     double TMP9_XOC, TMP10_XOC, TMP11_XOC, TMP12_XOC;
01282     double TMP13_XOC, TMP14_XOC, TMP15_XOC, TMP16_XOC;
01283     double TMP17_XOC, TMP18_XOC, TMP19_XOC, TMP20_XOC;
01284     double TMP21_XOC, TMP22_XOC, TMP23_XOC, TMP24_XOC;
01285     double TMP25_XOC, TMP26_XOC, TMP27_XOC;
01286
01287     double TMP1_XOE, TMP2_XOE, TMP3_XOE, TMP4_XOE;
01288     double TMP5_XOE, TMP6_XOE, TMP7_XOE, TMP8_XOE;
01289     double TMP9_XOE, TMP10_XOE, TMP11_XOE, TMP12_XOE;
01290
01291     double TMP1_XON, TMP2_XON, TMP3_XON, TMP4_XON;
01292     double TMP5_XON, TMP6_XON, TMP7_XON, TMP8_XON;
01293     double TMP9_XON, TMP10_XON, TMP11_XON, TMP12_XON;
01294
01295     double TMP1_XUC, TMP2_XUC, TMP3_XUC, TMP4_XUC;
01296     double TMP5_XUC, TMP6_XUC, TMP7_XUC, TMP8_XUC;
01297     double TMP9_XUC, TMP10_XUC, TMP11_XUC, TMP12_XUC;
01298
01299     double TMP1_XONE, TMP2_XONE, TMP3_XONE, TMP4_XONE;
01300     double TMP5_XONE, TMP6_XONE;
01301
01302     double TMP1_XONW, TMP2_XONW, TMP3_XONW, TMP4_XONW;
01303     double TMP5_XONW, TMP6_XONW;
01304
01305     double TMP1_XUE, TMP2_XUE, TMP3_XUE, TMP4_XUE;
01306     double TMP5_XUE, TMP6_XUE;
01307
01308     double TMP1_XUW, TMP2_XUW, TMP3_XUW, TMP4_XUW;
01309     double TMP5_XUW, TMP6_XUW;
01310
01311     double TMP1_XUN, TMP2_XUN, TMP3_XUN, TMP4_XUN;
01312     double TMP5_XUN, TMP6_XUN;
01313
01314     double TMP1_XUS, TMP2_XUS, TMP3_XUS, TMP4_XUS;
01315     double TMP5_XUS, TMP6_XUS;
01316
01317     double TMP1_XUNE, TMP2_XUNE, TMP1_XUNW, TMP2_XUNW;
01318     double TMP1_XUSE, TMP2_XUSE, TMP1_XUSW, TMP2_XUSW;
01319
01320     MAT3( oC, *nxf, *nyf, *nzf);
01321     MAT3( oE, *nxf, *nyf, *nzf);
01322     MAT3( oN, *nxf, *nyf, *nzf);
01323     MAT3( oNE, *nxf, *nyf, *nzf);
01324     MAT3( oNW, *nxf, *nyf, *nzf);
01325
01326     MAT3( uC, *nxf, *nyf, *nzf);
01327     MAT3( uE, *nxf, *nyf, *nzf);
01328     MAT3( uW, *nxf, *nyf, *nzf);
01329     MAT3( uN, *nxf, *nyf, *nzf);

```

```

01330     MAT3( uS, *nxf, *nyf, *nzf);
01331     MAT3( uNE, *nxf, *nyf, *nzf);
01332     MAT3( uNW, *nxf, *nyf, *nzf);
01333     MAT3( uSE, *nxf, *nyf, *nzf);
01334     MAT3( uSW, *nxf, *nyf, *nzf);
01335
01336     MAT3( XoC, *nx, *ny, *nz);
01337     MAT3( XoE, *nx, *ny, *nz);
01338     MAT3( XoN, *nx, *ny, *nz);
01339     MAT3( XoNE, *nx, *ny, *nz);
01340     MAT3( XoNW, *nx, *ny, *nz);
01341
01342     MAT3( XuC, *nx, *ny, *nz);
01343     MAT3( XuE, *nx, *ny, *nz);
01344     MAT3( XuW, *nx, *ny, *nz);
01345     MAT3( XuN, *nx, *ny, *nz);
01346     MAT3( XuS, *nx, *ny, *nz);
01347     MAT3( XuNE, *nx, *ny, *nz);
01348     MAT3( XuNW, *nx, *ny, *nz);
01349     MAT3( XuSE, *nx, *ny, *nz);
01350     MAT3( XuSW, *nx, *ny, *nz);
01351
01352     MAT3( oPC, *nx, *ny, *nz);
01353     MAT3( oPN, *nx, *ny, *nz);
01354     MAT3( oPS, *nx, *ny, *nz);
01355     MAT3( oPE, *nx, *ny, *nz);
01356     MAT3( oPW, *nx, *ny, *nz);
01357     MAT3( oPNE, *nx, *ny, *nz);
01358     MAT3( oPNW, *nx, *ny, *nz);
01359     MAT3( oPSE, *nx, *ny, *nz);
01360     MAT3( oPSW, *nx, *ny, *nz);
01361
01362     MAT3( uPC, *nx, *ny, *nz);
01363     MAT3( uPN, *nx, *ny, *nz);
01364     MAT3( uPS, *nx, *ny, *nz);
01365     MAT3( uPE, *nx, *ny, *nz);
01366     MAT3( uPW, *nx, *ny, *nz);
01367     MAT3( uPNE, *nx, *ny, *nz);
01368     MAT3( uPNW, *nx, *ny, *nz);
01369     MAT3( uPSE, *nx, *ny, *nz);
01370     MAT3( uPSW, *nx, *ny, *nz);
01371
01372     MAT3( dPC, *nx, *ny, *nz);
01373     MAT3( dPN, *nx, *ny, *nz);
01374     MAT3( dPS, *nx, *ny, *nz);
01375     MAT3( dPE, *nx, *ny, *nz);
01376     MAT3( dPW, *nx, *ny, *nz);
01377     MAT3( dPNE, *nx, *ny, *nz);
01378     MAT3( dPNW, *nx, *ny, *nz);
01379     MAT3( dPSE, *nx, *ny, *nz);
01380     MAT3( dPSW, *nx, *ny, *nz);
01381
01382     // define n and determine number of mesh points ***
01383     nxm1 = *nx - 1;
01384     nym1 = *ny - 1;
01385     nzm1 = *nz - 1;
01386
01387     //fprintf(data, "%s\n", PRINT_FUNC);
01388
01389     // Build the operator ***
01390     for(kk=2; kk<=*nz-1; kk++) {
01391         k = 2 * kk - 1;
01392
01393         for(jj=2; jj<=*ny-1; jj++) {
01394             j = 2 * jj - 1;
01395
01396             for(ii=2; ii<=*nx-1; ii++) {
01397                 i = 2 * ii - 1;
01398
01399                 // Index computations
01400                 im1 = i - 1;
01401                 ip1 = i + 1;
01402                 im2 = i - 2;
01403                 ip2 = i + 2;
01404                 jm1 = j - 1;
01405                 jp1 = j + 1;
01406                 jm2 = j - 2;
01407                 jp2 = j + 2;
01408                 km1 = k - 1;
01409                 kp1 = k + 1;
01410                 km2 = k - 2;

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```

01411         kp2 = k + 2;
01412         iim1 = ii - 1;
01413         iip1 = ii + 1;
01414         jjm1 = jj - 1;
01415         jjp1 = jj + 1;
01416         kkm1 = kk - 1;
01417         kkp1 = kk + 1;
01418
01419
01420
01421         /* *****
01422         * *** > oC;
01423         * *****/
01424
01425         // VAT3( XoC, ii,jj,kk) =
01426     TMP1_XOC =
01427         VAT3( oPN, ii,jj,kk) * (- VAT3( uNE, im1,j,kml) * VAT3( dPW, ii,jj,kk)
01428             - VAT3( oNE, im1,j,k) * VAT3( oPW, ii,jj,kk)
01429             - VAT3( uSW, i,jp1,k) * VAT3( uPW, ii,jj,kk)
01430             - VAT3( uE, im1,jp1,kml) * VAT3( dPNW, ii,jj,kk)
01431             - VAT3( oE, im1,jp1,k) * VAT3( oPNW, ii,jj,kk)
01432             - VAT3( uW, i,jp1,k) * VAT3( uPNW, ii,jj,kk)
01433             - VAT3( uN, i,j,kml) * VAT3( dPC, ii,jj,kk)
01434             - VAT3( oN, i,j,k) * VAT3( oPC, ii,jj,kk)
01435             - VAT3( uS, i,jp1,k) * VAT3( uPC, ii,jj,kk)
01436             - VAT3( uC, i,jp1,kml) * VAT3( dPN, ii,jj,kk)
01437             + VAT3( oC, i,jp1,k) * VAT3( oPN, ii,jj,kk)
01438             - VAT3( uC, i,jp1,k) * VAT3( uPN, ii,jj,kk)
01439             - VAT3( uNW, ip1,j,kml) * VAT3( dPE, ii,jj,kk)
01440             - VAT3( oNW, ip1,j,k) * VAT3( oPE, ii,jj,kk)
01441             - VAT3( uSE, i,jp1,k) * VAT3( uPE, ii,jj,kk)
01442             - VAT3( uW, ip1,jp1,kml) * VAT3( dPNE, ii,jj,kk)
01443             - VAT3( oE, i,jp1,k) * VAT3( oPNE, ii,jj,kk)
01444             - VAT3( uE, i,jp1,k) * VAT3( uPNE, ii,jj,kk));
01445
01446     TMP2_XOC =
01447         + VAT3( dPN, ii,jj,kk) * (- VAT3( oNE, im1,j,kml) * VAT3( dPW, ii,jj,kk)
01448             - VAT3( uSW, i,jp1,kml) * VAT3( oPW, ii,jj,kk)
01449             - VAT3( oE, im1,jp1,kml) * VAT3( dPNW, ii,jj,kk)
01450             - VAT3( uW, i,jp1,kml) * VAT3( oPNW, ii,jj,kk)
01451             - VAT3( oN, i,j,kml) * VAT3( dPC, ii,jj,kk)
01452             - VAT3( uS, i,jp1,kml) * VAT3( oPC, ii,jj,kk)
01453             + VAT3( oC, i,jp1,kml) * VAT3( dPN, ii,jj,kk)
01454             - VAT3( uC, i,jp1,kml) * VAT3( oPN, ii,jj,kk)
01455             - VAT3( oNW, ip1,j,kml) * VAT3( dPE, ii,jj,kk)
01456             - VAT3( uSE, i,jp1,kml) * VAT3( oPE, ii,jj,kk)
01457             - VAT3( oE, i,jp1,kml) * VAT3( dPNE, ii,jj,kk)
01458             - VAT3( uE, i,jp1,kml) * VAT3( oPNE, ii,jj,kk));
01459
01460     TMP3_XOC =
01461         + VAT3( dPC, ii,jj,kk) * (- VAT3( oNE, im1,jml,kml) * VAT3( dPSW, ii,jj,kk)
01462             - VAT3( uSW, i,j,kml) * VAT3( oPSW, ii,jj,kk)
01463             - VAT3( oE, im1,j,kml) * VAT3( dPW, ii,jj,kk)
01464             - VAT3( uW, i,j,kml) * VAT3( oPW, ii,jj,kk)
01465             - VAT3( oNW, i,j,kml) * VAT3( dPNW, ii,jj,kk)
01466             - VAT3( uNW, i,j,kml) * VAT3( oPNW, ii,jj,kk)
01467             - VAT3( oN, i,jml,kml) * VAT3( dPS, ii,jj,kk)
01468             - VAT3( uS, i,j,kml) * VAT3( oPS, ii,jj,kk)
01469             + VAT3( oC, i,j,kml) * VAT3( dPC, ii,jj,kk)
01470             - VAT3( uC, i,j,kml) * VAT3( oPC, ii,jj,kk)
01471             - VAT3( oN, i,j,kml) * VAT3( dPN, ii,jj,kk)
01472             - VAT3( uN, i,j,kml) * VAT3( oPN, ii,jj,kk)
01473             - VAT3( oNW, ip1,jml,kml) * VAT3( dPSE, ii,jj,kk)
01474             - VAT3( uSE, i,j,kml) * VAT3( oPSE, ii,jj,kk)
01475             - VAT3( oE, i,j,kml) * VAT3( dPE, ii,jj,kk)
01476             - VAT3( uE, i,j,kml) * VAT3( oPE, ii,jj,kk)
01477             - VAT3( oNE, i,j,kml) * VAT3( dPNE, ii,jj,kk)
01478             - VAT3( uNE, i,j,kml) * VAT3( oPNE, ii,jj,kk));
01479
01480     TMP4_XOC =
01481         + VAT3( uPC, ii,jj,kk) * (- VAT3( uNE, im1,jml,k) * VAT3( oPSW, ii,jj,kk)
01482             - VAT3( oNE, im1,jml,kp1) * VAT3( uPSW, ii,jj,kk)
01483             - VAT3( uE, im1,j,k) * VAT3( oPW, ii,jj,kk)
01484             - VAT3( oE, im1,j,kp1) * VAT3( uPW, ii,jj,kk)
01485             - VAT3( uSE, im1,jp1,k) * VAT3( oPNW, ii,jj,kk)
01486             - VAT3( oNW, i,j,kp1) * VAT3( uPNW, ii,jj,kk)
01487             - VAT3( uN, i,jml,k) * VAT3( oPS, ii,jj,kk)
01488             - VAT3( oN, i,jml,kp1) * VAT3( uPS, ii,jj,kk)
01489             - VAT3( uC, i,j,k) * VAT3( oPC, ii,jj,kk)
01490             + VAT3( oC, i,j,kp1) * VAT3( uPC, ii,jj,kk)
01491             - VAT3( uS, i,jp1,k) * VAT3( oPN, ii,jj,kk)

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01492             - VAT3( oN, i, j, kp1) * VAT3( uPN, ii, jj, kk)
01493             - VAT3( uNW, ip1, jml, k) * VAT3( oPSE, ii, jj, kk)
01494             - VAT3( oNW, ip1, jml, kp1) * VAT3( uPSE, ii, jj, kk)
01495             - VAT3( uW, ip1, j, k) * VAT3( oPE, ii, jj, kk)
01496             - VAT3( oE, i, j, kp1) * VAT3( uPE, ii, jj, kk)
01497             - VAT3( uSW, ip1, jpl, k) * VAT3( oPNE, ii, jj, kk)
01498             - VAT3( oNE, i, j, kp1) * VAT3( uPNE, ii, jj, kk));
01499
01500 TMP5_XOC =
01501     + VAT3( oPC, ii, jj, kk) * (- VAT3( uW, ip1, j, kml) * VAT3( dPE, ii, jj, kk)
01502     - VAT3( oE, im1, j, k) * VAT3( oPW, ii, jj, kk)
01503     - VAT3( uSE, im1, jpl, kml) * VAT3( dPNW, ii, jj, kk)
01504     - VAT3( uNE, im1, jml, kml) * VAT3( dPSW, ii, jj, kk)
01505     - VAT3( uN, i, jml, kml) * VAT3( dPS, ii, jj, kk)
01506     - VAT3( oNE, im1, jml, k) * VAT3( oPSW, ii, jj, kk)
01507     - VAT3( uE, im1, j, kml) * VAT3( dPW, ii, jj, kk)
01508     - VAT3( oNW, ip1, jml, k) * VAT3( oPSE, ii, jj, kk)
01509     - VAT3( uC, i, j, kml) * VAT3( dPC, ii, jj, kk)
01510     - VAT3( uNW, ip1, jml, kml) * VAT3( dPSE, ii, jj, kk)
01511     - VAT3( uSW, ip1, jpl, kml) * VAT3( dPNE, ii, jj, kk)
01512     - VAT3( uS, i, jpl, kml) * VAT3( dPN, ii, jj, kk) - VAT3( oN, i, jml, k) * VAT3( oPS, ii, jj, kk)
01513     - VAT3( uNE, i, j, k) * VAT3( uPNE, ii, jj, kk) - VAT3( oNE, i, j, k) * VAT3( oPNE, ii, jj, kk)
01514     - VAT3( uE, i, j, k) * VAT3( uPE, ii, jj, kk) - VAT3( uSE, i, j, k) * VAT3( uPSE, ii, jj, kk)
01515     - VAT3( oN, i, j, k) * VAT3( oPN, ii, jj, kk) - VAT3( oE, i, j, k) * VAT3( oPE, ii, jj, kk)
01516     - VAT3( uS, i, j, k) * VAT3( uPS, ii, jj, kk) + VAT3( oC, i, j, k) * VAT3( oPC, ii, jj, kk)
01517     - VAT3( uSW, i, j, k) * VAT3( uPSW, ii, jj, kk) - VAT3( uN, i, j, k) * VAT3( uPN, ii, jj, kk)
01518     - VAT3( uC, i, j, k) * VAT3( uPC, ii, jj, kk) - VAT3( uW, i, j, k) * VAT3( uPW, ii, jj, kk)
01519     - VAT3( oNW, i, j, k) * VAT3( oPNW, ii, jj, kk) - VAT3( uNW, i, j, k) * VAT3( uPNW, ii, jj, kk));
01520
01521 TMP6_XOC =
01522     + VAT3( uPS, ii, jj, kk) * (- VAT3( uE, im1, jml, k) * VAT3( oPSW, ii, jj, kk)
01523     - VAT3( oE, im1, jml, kp1) * VAT3( uPSW, ii, jj, kk)
01524     - VAT3( uSE, im1, j, k) * VAT3( oPW, ii, jj, kk)
01525     - VAT3( oNW, i, jml, kp1) * VAT3( uPW, ii, jj, kk)
01526     - VAT3( uC, i, jml, k) * VAT3( oPS, ii, jj, kk)
01527     + VAT3( oC, i, jml, kp1) * VAT3( uPS, ii, jj, kk)
01528     - VAT3( uS, i, j, k) * VAT3( oPC, ii, jj, kk)
01529     - VAT3( oN, i, jml, kp1) * VAT3( uPC, ii, jj, kk)
01530     - VAT3( uW, ip1, jml, k) * VAT3( oPSE, ii, jj, kk)
01531     - VAT3( oE, i, jml, kp1) * VAT3( uPSE, ii, jj, kk)
01532     - VAT3( uSW, ip1, j, k) * VAT3( oPE, ii, jj, kk)
01533     - VAT3( oNE, i, jml, kp1) * VAT3( uPE, ii, jj, kk));
01534
01535 TMP7_XOC =
01536     + VAT3( oPS, ii, jj, kk) * (- VAT3( uE, im1, jml, kml) * VAT3( dPSW, ii, jj, kk)
01537     - VAT3( oE, im1, jml, k) * VAT3( oPSW, ii, jj, kk)
01538     - VAT3( uW, i, jml, k) * VAT3( uPSW, ii, jj, kk)
01539     - VAT3( uSE, im1, j, kml) * VAT3( dPW, ii, jj, kk)
01540     - VAT3( oNW, i, jml, k) * VAT3( oPW, ii, jj, kk)
01541     - VAT3( uNW, i, jml, k) * VAT3( uPW, ii, jj, kk)
01542     - VAT3( uC, i, jml, kml) * VAT3( dPS, ii, jj, kk)
01543     + VAT3( oC, i, jml, k) * VAT3( oPS, ii, jj, kk)
01544     - VAT3( uC, i, jml, k) * VAT3( uPS, ii, jj, kk)
01545     - VAT3( uS, i, j, kml) * VAT3( dPC, ii, jj, kk)
01546     - VAT3( oN, i, jml, k) * VAT3( oPC, ii, jj, kk)
01547     - VAT3( uN, i, jml, k) * VAT3( uPC, ii, jj, kk)
01548     - VAT3( uW, ip1, jml, kml) * VAT3( dPSE, ii, jj, kk)
01549     - VAT3( oE, i, jml, k) * VAT3( oPSE, ii, jj, kk)
01550     - VAT3( uE, i, jml, k) * VAT3( uPSE, ii, jj, kk)
01551     - VAT3( uSW, ip1, j, kml) * VAT3( dPE, ii, jj, kk)
01552     - VAT3( oNE, i, jml, k) * VAT3( oPE, ii, jj, kk)
01553     - VAT3( uNE, i, jml, k) * VAT3( uPE, ii, jj, kk));
01554
01555 TMP8_XOC =
01556     + VAT3( dPS, ii, jj, kk) * (- VAT3( oE, im1, jml, kml) * VAT3( dPSW, ii, jj, kk)
01557     - VAT3( uW, i, jml, kml) * VAT3( oPSW, ii, jj, kk)
01558     - VAT3( oNW, i, jml, kml) * VAT3( dPW, ii, jj, kk)
01559     - VAT3( uNW, i, jml, kml) * VAT3( oPW, ii, jj, kk)
01560     + VAT3( oC, i, jml, kml) * VAT3( dPS, ii, jj, kk)
01561     - VAT3( uC, i, jml, kml) * VAT3( oPS, ii, jj, kk)
01562     - VAT3( oN, i, jml, kml) * VAT3( dPC, ii, jj, kk)
01563     - VAT3( uN, i, jml, kml) * VAT3( oPC, ii, jj, kk)
01564     - VAT3( oE, i, jml, kml) * VAT3( dPSE, ii, jj, kk)
01565     - VAT3( uE, i, jml, kml) * VAT3( oPSE, ii, jj, kk)
01566     - VAT3( oNE, i, jml, kml) * VAT3( dPE, ii, jj, kk)
01567     - VAT3( uNE, i, jml, kml) * VAT3( oPE, ii, jj, kk));
01568
01569 TMP9_XOC =
01570     + VAT3( uPNW, ii, jj, kk) * (- VAT3( uN, im1, j, k) * VAT3( oPW, ii, jj, kk)
01571     - VAT3( oN, im1, j, kp1) * VAT3( uPW, ii, jj, kk)
01572     - VAT3( uC, im1, jpl, k) * VAT3( oPNW, ii, jj, kk)

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01573             + VAT3( oC, iml,jpl,kpl) * VAT3(uPNW, ii,jj,kk)
01574             - VAT3( uNW, i,j,k) * VAT3( oPC, ii,jj,kk)
01575             - VAT3( oNW, i,j,kpl) * VAT3( uPC, ii,jj,kk)
01576             - VAT3( uW, i,jpl,k) * VAT3( oPN, ii,jj,kk)
01577             - VAT3( oE, iml,jpl,kpl) * VAT3( uPN, ii,jj,kk));
01578
01579 TMP10_XOC =
01580     + VAT3(oPNW, ii,jj,kk) * (- VAT3( uN, iml,j,kml) * VAT3( dPW, ii,jj,kk)
01581     - VAT3( oN, iml,j,k) * VAT3( oPW, ii,jj,kk)
01582     - VAT3( uS, iml,jpl,k) * VAT3( uPW, ii,jj,kk)
01583     - VAT3( uC, iml,jpl,kml) * VAT3(dPNW, ii,jj,kk)
01584     + VAT3( oC, iml,jpl,k) * VAT3(oPNW, ii,jj,kk)
01585     - VAT3( uC, iml,jpl,k) * VAT3(uPNW, ii,jj,kk)
01586     - VAT3( uNW, i,j,kml) * VAT3( dPC, ii,jj,kk)
01587     - VAT3( oNW, i,j,k) * VAT3( oPC, ii,jj,kk)
01588     - VAT3( uSE, iml,jpl,k) * VAT3( uPC, ii,jj,kk)
01589     - VAT3( uW, i,jpl,kml) * VAT3( dPN, ii,jj,kk)
01590     - VAT3( oE, iml,jpl,k) * VAT3( oPN, ii,jj,kk)
01591     - VAT3( uE, iml,jpl,k) * VAT3( uPN, ii,jj,kk));
01592
01593 TMP11_XOC =
01594     + VAT3( uPW, ii,jj,kk) * (- VAT3( uN, iml,jml,k) * VAT3(oPSW, ii,jj,kk)
01595     - VAT3( oN, iml,jml,kpl) * VAT3(uPSW, ii,jj,kk)
01596     - VAT3( uC, iml,j,k) * VAT3( oPW, ii,jj,kk)
01597     + VAT3( oC, iml,j,kpl) * VAT3( uPW, ii,jj,kk)
01598     - VAT3( uS, iml,jpl,k) * VAT3(oPNW, ii,jj,kk)
01599     - VAT3( oN, iml,j,kpl) * VAT3(uPNW, ii,jj,kk)
01600     - VAT3( uNW, i,jml,k) * VAT3( oPS, ii,jj,kk)
01601     - VAT3( oNW, i,jml,kpl) * VAT3( uPS, ii,jj,kk)
01602     - VAT3( uW, i,j,k) * VAT3( oPC, ii,jj,kk)
01603     - VAT3( oE, iml,j,kpl) * VAT3( uPC, ii,jj,kk)
01604     - VAT3( uSW, i,jpl,k) * VAT3( oPN, ii,jj,kk)
01605     - VAT3( oNE, iml,j,kpl) * VAT3( uPN, ii,jj,kk));
01606
01607 TMP12_XOC =
01608     + VAT3(dPNW, ii,jj,kk) * (- VAT3( oN, iml,j,kml) * VAT3( dPW, ii,jj,kk)
01609     - VAT3( uS, iml,jpl,kml) * VAT3( oPW, ii,jj,kk)
01610     + VAT3( oC, iml,jpl,kml) * VAT3(dPNW, ii,jj,kk)
01611     - VAT3( uC, iml,jpl,kml) * VAT3(oPNW, ii,jj,kk)
01612     - VAT3( oNW, i,j,kml) * VAT3( dPC, ii,jj,kk)
01613     - VAT3( uSE, iml,jpl,kml) * VAT3( oPC, ii,jj,kk)
01614     - VAT3( oE, iml,jpl,kml) * VAT3( dPN, ii,jj,kk)
01615     - VAT3( uE, iml,jpl,kml) * VAT3( oPN, ii,jj,kk));
01616
01617 TMP13_XOC =
01618     + VAT3( oPW, ii,jj,kk) * (- VAT3( uN, iml,jml,kml) * VAT3(dPSW, ii,jj,kk)
01619     - VAT3( oN, iml,jml,k) * VAT3(oPSW, ii,jj,kk)
01620     - VAT3( uS, iml,j,k) * VAT3(uPSW, ii,jj,kk)
01621     - VAT3( uC, iml,j,kml) * VAT3( dPW, ii,jj,kk)
01622     + VAT3( oC, iml,j,k) * VAT3( oPW, ii,jj,kk)
01623     - VAT3( uC, iml,j,k) * VAT3( uPW, ii,jj,kk)
01624     - VAT3( uS, iml,jpl,kml) * VAT3(dPNW, ii,jj,kk)
01625     - VAT3( oN, iml,j,k) * VAT3(oPNW, ii,jj,kk)
01626     - VAT3( uN, iml,j,k) * VAT3(uPNW, ii,jj,kk)
01627     - VAT3( uNW, i,jml,kml) * VAT3( dPS, ii,jj,kk)
01628     - VAT3( oNW, i,jml,k) * VAT3( oPS, ii,jj,kk)
01629     - VAT3( uSE, iml,j,k) * VAT3( uPS, ii,jj,kk)
01630     - VAT3( uW, i,j,kml) * VAT3( dPC, ii,jj,kk)
01631     - VAT3( oE, iml,j,k) * VAT3( oPC, ii,jj,kk)
01632     - VAT3( uE, iml,j,k) * VAT3( uPC, ii,jj,kk)
01633     - VAT3( uSW, i,jpl,kml) * VAT3( dPN, ii,jj,kk)
01634     - VAT3( oNE, iml,j,k) * VAT3( oPN, ii,jj,kk)
01635     - VAT3( uNE, iml,j,k) * VAT3( uPN, ii,jj,kk));
01636
01637 TMP14_XOC =
01638     + VAT3(uPSW, ii,jj,kk) * (- VAT3( uC, iml,jml,k) * VAT3(oPSW, ii,jj,kk)
01639     + VAT3( oC, iml,jml,kpl) * VAT3(uPSW, ii,jj,kk)
01640     - VAT3( uS, iml,j,k) * VAT3( oPW, ii,jj,kk)
01641     - VAT3( oN, iml,jml,kpl) * VAT3( uPW, ii,jj,kk)
01642     - VAT3( uW, i,jml,k) * VAT3( oPS, ii,jj,kk)
01643     - VAT3( oE, iml,jml,kpl) * VAT3( uPS, ii,jj,kk)
01644     - VAT3( uSW, i,j,k) * VAT3( oPC, ii,jj,kk)
01645     - VAT3( oNE, iml,jml,kpl) * VAT3( uPC, ii,jj,kk));
01646
01647 TMP15_XOC =
01648     + VAT3(oPSW, ii,jj,kk) * (- VAT3( uC, iml,jml,kml) * VAT3(dPSW, ii,jj,kk)
01649     + VAT3( oC, iml,jml,k) * VAT3(oPSW, ii,jj,kk)
01650     - VAT3( uC, iml,jml,k) * VAT3(uPSW, ii,jj,kk)
01651     - VAT3( uS, iml,j,kml) * VAT3( dPW, ii,jj,kk)
01652     - VAT3( oN, iml,jml,k) * VAT3( oPW, ii,jj,kk)
01653     - VAT3( uN, iml,jml,k) * VAT3( uPW, ii,jj,kk)

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01654             - VAT3( uW, i, jml, kml) * VAT3( dPS, ii, jj, kk)
01655             - VAT3( oE, iml, jml, k) * VAT3( oPS, ii, jj, kk)
01656             - VAT3( uE, iml, jml, k) * VAT3( uPS, ii, jj, kk)
01657             - VAT3( uSW, i, j, kml) * VAT3( dPC, ii, jj, kk)
01658             - VAT3( oNE, iml, jml, k) * VAT3( oPC, ii, jj, kk)
01659             - VAT3( uNE, iml, jml, k) * VAT3( uPC, ii, jj, kk));
01660
01661 TMP16_XOC =
01662     + VAT3( dPW, ii, jj, kk) * (- VAT3( oN, iml, jml, kml) * VAT3( dPSW, ii, jj, kk)
01663     - VAT3( uS, iml, j, kml) * VAT3( oPSW, ii, jj, kk)
01664     + VAT3( oC, iml, j, kml) * VAT3( dPW, ii, jj, kk)
01665     - VAT3( uC, iml, j, kml) * VAT3( oPW, ii, jj, kk)
01666     - VAT3( oN, iml, j, kml) * VAT3( dPNW, ii, jj, kk)
01667     - VAT3( uN, iml, j, kml) * VAT3( oPNW, ii, jj, kk)
01668     - VAT3( oNW, i, jml, kml) * VAT3( dPS, ii, jj, kk)
01669     - VAT3( uSE, iml, j, kml) * VAT3( oPS, ii, jj, kk)
01670     - VAT3( oE, iml, j, kml) * VAT3( dPC, ii, jj, kk)
01671     - VAT3( uE, iml, j, kml) * VAT3( oPC, ii, jj, kk)
01672     - VAT3( oNE, iml, j, kml) * VAT3( dPN, ii, jj, kk)
01673     - VAT3( uNE, iml, j, kml) * VAT3( oPN, ii, jj, kk));
01674
01675 TMP17_XOC =
01676     + VAT3( uPNE, ii, jj, kk) * (- VAT3( uNE, i, j, k) * VAT3( oPC, ii, jj, kk)
01677     - VAT3( oNE, i, j, kpl) * VAT3( uPC, ii, jj, kk)
01678     - VAT3( uE, i, jpl, k) * VAT3( oPN, ii, jj, kk)
01679     - VAT3( oE, i, jpl, kpl) * VAT3( uPN, ii, jj, kk)
01680     - VAT3( uN, ipl, j, k) * VAT3( oPE, ii, jj, kk)
01681     - VAT3( oN, ipl, j, kpl) * VAT3( uPE, ii, jj, kk)
01682     - VAT3( uC, ipl, jpl, k) * VAT3( oPNE, ii, jj, kk)
01683     + VAT3( oC, ipl, jpl, kpl) * VAT3( uPNE, ii, jj, kk));
01684
01685 TMP18_XOC =
01686     + VAT3( uPE, ii, jj, kk) * (- VAT3( uNE, i, jml, k) * VAT3( oPS, ii, jj, kk)
01687     - VAT3( oNE, i, jml, kpl) * VAT3( uPS, ii, jj, kk)
01688     - VAT3( uE, i, j, k) * VAT3( oPC, ii, jj, kk)
01689     - VAT3( oE, i, j, kpl) * VAT3( uPC, ii, jj, kk)
01690     - VAT3( uSE, i, jpl, k) * VAT3( oPN, ii, jj, kk)
01691     - VAT3( oNW, ipl, j, kpl) * VAT3( uPN, ii, jj, kk)
01692     - VAT3( uN, ipl, jml, k) * VAT3( oPSE, ii, jj, kk)
01693     - VAT3( oN, ipl, jml, kpl) * VAT3( uPSE, ii, jj, kk)
01694     - VAT3( uC, ipl, j, k) * VAT3( oPE, ii, jj, kk)
01695     + VAT3( oC, ipl, j, kpl) * VAT3( uPE, ii, jj, kk)
01696     - VAT3( uS, ipl, jpl, k) * VAT3( oPNE, ii, jj, kk)
01697     - VAT3( oN, ipl, j, kpl) * VAT3( uPNE, ii, jj, kk));
01698
01699 TMP19_XOC =
01700     + VAT3( dPNE, ii, jj, kk) * (- VAT3( oNE, i, j, kml) * VAT3( dPC, ii, jj, kk)
01701     - VAT3( uSW, ipl, jpl, kml) * VAT3( oPC, ii, jj, kk)
01702     - VAT3( oE, i, jpl, kml) * VAT3( dPN, ii, jj, kk)
01703     - VAT3( uW, ipl, jpl, kml) * VAT3( oPN, ii, jj, kk)
01704     - VAT3( oN, ipl, j, kml) * VAT3( dPE, ii, jj, kk)
01705     - VAT3( uS, ipl, jpl, kml) * VAT3( oPE, ii, jj, kk)
01706     + VAT3( oC, ipl, jpl, kml) * VAT3( dPNE, ii, jj, kk)
01707     - VAT3( uC, ipl, jpl, kml) * VAT3( oPNE, ii, jj, kk));
01708
01709 TMP20_XOC =
01710     + VAT3( oPNE, ii, jj, kk) * (- VAT3( uNE, i, j, kml) * VAT3( dPC, ii, jj, kk)
01711     - VAT3( oNE, i, j, k) * VAT3( oPC, ii, jj, kk)
01712     - VAT3( uSW, ipl, jpl, k) * VAT3( uPC, ii, jj, kk)
01713     - VAT3( uE, i, jpl, kml) * VAT3( dPN, ii, jj, kk)
01714     - VAT3( oE, i, jpl, k) * VAT3( oPN, ii, jj, kk)
01715     - VAT3( uW, ipl, jpl, k) * VAT3( uPN, ii, jj, kk)
01716     - VAT3( uN, ipl, j, kml) * VAT3( dPE, ii, jj, kk)
01717     - VAT3( oN, ipl, j, k) * VAT3( oPE, ii, jj, kk)
01718     - VAT3( uS, ipl, jpl, k) * VAT3( uPE, ii, jj, kk)
01719     - VAT3( uC, ipl, jpl, kml) * VAT3( dPNE, ii, jj, kk)
01720     + VAT3( oC, ipl, jpl, k) * VAT3( oPNE, ii, jj, kk)
01721     - VAT3( uC, ipl, jpl, k) * VAT3( uPNE, ii, jj, kk));
01722
01723 TMP21_XOC =
01724     + VAT3( oPSE, ii, jj, kk) * (- VAT3( uE, i, jml, kml) * VAT3( dPS, ii, jj, kk)
01725     - VAT3( oE, i, jml, k) * VAT3( oPS, ii, jj, kk)
01726     - VAT3( uW, ipl, jml, k) * VAT3( uPS, ii, jj, kk)
01727     - VAT3( uSE, i, j, kml) * VAT3( dPC, ii, jj, kk)
01728     - VAT3( oNW, ipl, jml, k) * VAT3( oPC, ii, jj, kk)
01729     - VAT3( uNW, ipl, jml, k) * VAT3( uPC, ii, jj, kk)
01730     - VAT3( uC, ipl, jml, kml) * VAT3( dPSE, ii, jj, kk)
01731     + VAT3( oC, ipl, jml, k) * VAT3( oPSE, ii, jj, kk)
01732     - VAT3( uC, ipl, jml, k) * VAT3( uPSE, ii, jj, kk)
01733     - VAT3( uS, ipl, j, kml) * VAT3( dPE, ii, jj, kk)
01734     - VAT3( oN, ipl, jml, k) * VAT3( oPE, ii, jj, kk)

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01735             - VAT3( uN, ip1,jm1,k) * VAT3( uPE, ii,jj,kk));
01736
01737 TMP22_XOC =
01738     + VAT3(dPSE, ii,jj,kk) * (- VAT3( oE, i,jm1,km1) * VAT3( dPS, ii,jj,kk)
01739     - VAT3( uW, ip1,jm1,km1) * VAT3( oPS, ii,jj,kk)
01740     - VAT3( oNW, ip1,jm1,km1) * VAT3( dPC, ii,jj,kk)
01741     - VAT3( uNW, ip1,jm1,km1) * VAT3( oPC, ii,jj,kk)
01742     + VAT3( oC, ip1,jm1,km1) * VAT3(dPSE, ii,jj,kk)
01743     - VAT3( uC, ip1,jm1,km1) * VAT3(oPSE, ii,jj,kk)
01744     - VAT3( oN, ip1,jm1,km1) * VAT3( dPE, ii,jj,kk)
01745     - VAT3( uN, ip1,jm1,km1) * VAT3( oPE, ii,jj,kk));
01746
01747 TMP23_XOC =
01748     + VAT3(uPSE, ii,jj,kk) * (- VAT3( uE, i,jm1,k) * VAT3( oPS, ii,jj,kk)
01749     - VAT3( oE, i,jm1,kp1) * VAT3( uPS, ii,jj,kk)
01750     - VAT3( uSE, i,j,k) * VAT3( oPC, ii,jj,kk)
01751     - VAT3( oNW, ip1,jm1,kp1) * VAT3( uPC, ii,jj,kk)
01752     - VAT3( uC, ip1,jm1,k) * VAT3(oPSE, ii,jj,kk)
01753     + VAT3( oC, ip1,jm1,kp1) * VAT3(uPSE, ii,jj,kk)
01754     - VAT3( uS, ip1,j,k) * VAT3( oPE, ii,jj,kk)
01755     - VAT3( oN, ip1,jm1,kp1) * VAT3( uPE, ii,jj,kk));
01756
01757 TMP24_XOC =
01758     + VAT3( oPE, ii,jj,kk) * (- VAT3( uNE, i,jm1,km1) * VAT3( dPS, ii,jj,kk)
01759     - VAT3( oNE, i,jm1,k) * VAT3( oPS, ii,jj,kk)
01760     - VAT3( uSW, ip1,j,k) * VAT3( uPS, ii,jj,kk)
01761     - VAT3( uE, i,j,km1) * VAT3( dPC, ii,jj,kk)
01762     - VAT3( oE, i,j,k) * VAT3( oPC, ii,jj,kk)
01763     - VAT3( uW, ip1,j,k) * VAT3( uPC, ii,jj,kk)
01764     - VAT3( uSE, i,jp1,km1) * VAT3( dPN, ii,jj,kk)
01765     - VAT3( oNW, ip1,j,k) * VAT3( oPN, ii,jj,kk)
01766     - VAT3( uNW, ip1,j,k) * VAT3( uPN, ii,jj,kk)
01767     - VAT3( uN, ip1,jm1,km1) * VAT3(dPSE, ii,jj,kk)
01768     - VAT3( oN, ip1,jm1,k) * VAT3(oPSE, ii,jj,kk)
01769     - VAT3( uS, ip1,j,k) * VAT3(uPSE, ii,jj,kk)
01770     - VAT3( uC, ip1,j,km1) * VAT3( dPE, ii,jj,kk)
01771     + VAT3( oC, ip1,j,k) * VAT3( oPE, ii,jj,kk)
01772     - VAT3( uC, ip1,j,k) * VAT3( uPE, ii,jj,kk)
01773     - VAT3( uS, ip1,jp1,km1) * VAT3(dPNE, ii,jj,kk)
01774     - VAT3( oN, ip1,j,k) * VAT3(oPNE, ii,jj,kk)
01775     - VAT3( uN, ip1,j,k) * VAT3(uPNE, ii,jj,kk));
01776
01777 TMP25_XOC =
01778     + VAT3( dPE, ii,jj,kk) * (- VAT3( oNE, i,jm1,km1) * VAT3( dPS, ii,jj,kk)
01779     - VAT3( uSW, ip1,j,km1) * VAT3( oPS, ii,jj,kk)
01780     - VAT3( oE, i,j,km1) * VAT3( dPC, ii,jj,kk)
01781     - VAT3( uW, ip1,j,km1) * VAT3( oPC, ii,jj,kk)
01782     - VAT3( oNW, ip1,j,km1) * VAT3( dPN, ii,jj,kk)
01783     - VAT3( uNW, ip1,j,km1) * VAT3( oPN, ii,jj,kk)
01784     - VAT3( oN, ip1,jm1,km1) * VAT3(dPSE, ii,jj,kk)
01785     - VAT3( uS, ip1,j,km1) * VAT3(oPSE, ii,jj,kk)
01786     + VAT3( oC, ip1,j,km1) * VAT3( dPE, ii,jj,kk)
01787     - VAT3( uC, ip1,j,km1) * VAT3( oPE, ii,jj,kk)
01788     - VAT3( oN, ip1,j,km1) * VAT3(dPNE, ii,jj,kk)
01789     - VAT3( uN, ip1,j,km1) * VAT3(oPNE, ii,jj,kk));
01790
01791 TMP26_XOC =
01792     + VAT3( uPN, ii,jj,kk) * (- VAT3( uNE, im1,j,k) * VAT3( oPW, ii,jj,kk)
01793     - VAT3( oNE, im1,j,kp1) * VAT3( uPW, ii,jj,kk)
01794     - VAT3( uE, im1,jp1,k) * VAT3(oPNW, ii,jj,kk)
01795     - VAT3( oE, im1,jp1,kp1) * VAT3(uPNW, ii,jj,kk)
01796     - VAT3( uN, i,j,k) * VAT3( oPC, ii,jj,kk)
01797     - VAT3( oN, i,j,kp1) * VAT3( uPC, ii,jj,kk)
01798     - VAT3( uC, i,jp1,k) * VAT3( oPN, ii,jj,kk)
01799     + VAT3( oC, i,jp1,kp1) * VAT3( uPN, ii,jj,kk)
01800     - VAT3( uNW, ip1,j,k) * VAT3( oPE, ii,jj,kk)
01801     - VAT3( oNW, ip1,j,kp1) * VAT3( uPE, ii,jj,kk)
01802     - VAT3( uW, ip1,jp1,k) * VAT3(oPNE, ii,jj,kk)
01803     - VAT3( oE, i,jp1,kp1) * VAT3(uPNE, ii,jj,kk));
01804
01805 TMP27_XOC =
01806     + VAT3(dPSW, ii,jj,kk) * ( VAT3( oC, im1,jm1,km1) * VAT3(dPSW, ii,jj,kk)
01807     - VAT3( uC, im1,jm1,km1) * VAT3(oPSW, ii,jj,kk)
01808     - VAT3( oN, im1,jm1,km1) * VAT3( dPW, ii,jj,kk)
01809     - VAT3( uN, im1,jm1,km1) * VAT3( oPW, ii,jj,kk)
01810     - VAT3( oE, im1,jm1,km1) * VAT3( dPS, ii,jj,kk)
01811     - VAT3( uE, im1,jm1,km1) * VAT3( oPS, ii,jj,kk)
01812     - VAT3( oNE, im1,jm1,km1) * VAT3( dPC, ii,jj,kk)
01813     - VAT3( uNE, im1,jm1,km1) * VAT3( oPC, ii,jj,kk));
01814
01815 VAT3( XoC, ii,jj,kk) = TMP1_XOC + TMP2_XOC + TMP3_XOC + TMP4_XOC

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01816      + TMP5_XOC + TMP6_XOC + TMP7_XOC + TMP8_XOC + TMP9_XOC
01817      + TMP10_XOC + TMP11_XOC + TMP12_XOC + TMP13_XOC + TMP14_XOC
01818      + TMP15_XOC + TMP16_XOC + TMP17_XOC + TMP18_XOC + TMP19_XOC
01819      + TMP20_XOC + TMP21_XOC + TMP22_XOC + TMP23_XOC + TMP24_XOC
01820      + TMP25_XOC + TMP26_XOC + TMP27_XOC;
01821
01822      //fprintf(data, "%19.12E\n", VAT3(XoC, ii, jj, kk));
01823
01824      /* *****
01825      * *** > OE;
01826      * *****/
01827
01828      // VAT3( XoE, ii,jj,kk) =
01829      TMP1_XOE =
01830      - VAT3( dPS, ii,jj,kk) * ( - VAT3( oE, i,jm1,km1) * VAT3(dPSW, iip1,jj,kk)
01831      - VAT3( uE, i,jm1,km1) * VAT3(oPSW, iip1,jj,kk)
01832      - VAT3( oNE, i,jm1,km1) * VAT3( dPW, iip1,jj,kk)
01833      - VAT3( uNE, i,jm1,km1) * VAT3( oPW, iip1,jj,kk))
01834
01835      - VAT3( oPS, ii,jj,kk) * ( - VAT3( uW, ip1,jm1,km1) * VAT3(dPSW, iip1,jj,kk)
01836      - VAT3( oE, i,jm1,k) * VAT3(oPSW, iip1,jj,kk)
01837      - VAT3( uE, i,jm1,k) * VAT3(uPSW, iip1,jj,kk)
01838      - VAT3( uSW, ip1,j,km1) * VAT3( dPW, iip1,jj,kk)
01839      - VAT3( oNE, i,jm1,k) * VAT3( oPW, iip1,jj,kk)
01840      - VAT3( uNE, i,jm1,k) * VAT3( uPW, iip1,jj,kk))
01841
01842      - VAT3( uPS, ii,jj,kk) * ( - VAT3( uW, ip1,jm1,k) * VAT3(oPSW, iip1,jj,kk)
01843      - VAT3( oE, i,jm1,kp1) * VAT3(uPSW, iip1,jj,kk)
01844      - VAT3( uSW, ip1,j,k) * VAT3( oPW, iip1,jj,kk)
01845      - VAT3( oNE, i,jm1,kp1) * VAT3( uPW, iip1,jj,kk));
01846
01847      TMP2_XOE =
01848      - VAT3( dPC, ii,jj,kk) * ( - VAT3( oNW, ip1,jm1,km1) * VAT3(dPSW, iip1,jj,kk)
01849      - VAT3( uSE, i,j,km1) * VAT3(oPSW, iip1,jj,kk)
01850      - VAT3( oE, i,j,km1) * VAT3( dPW, iip1,jj,kk)
01851      - VAT3( uE, i,j,km1) * VAT3( oPW, iip1,jj,kk)
01852      - VAT3( oNE, i,j,km1) * VAT3(dPNW, iip1,jj,kk)
01853      - VAT3( uNE, i,j,km1) * VAT3(oPNW, iip1,jj,kk))
01854
01855      - VAT3( oPC, ii,jj,kk) * ( - VAT3( uNW, ip1,jm1,km1) * VAT3(dPSW, iip1,jj,kk)
01856      - VAT3( oNW, ip1,jm1,k) * VAT3(oPSW, iip1,jj,kk)
01857      - VAT3( uSE, i,j,k) * VAT3(uPSW, iip1,jj,kk)
01858      - VAT3( uW, ip1,j,km1) * VAT3( dPW, iip1,jj,kk)
01859      - VAT3( oE, i,j,k) * VAT3( oPW, iip1,jj,kk)
01860      - VAT3( uE, i,j,k) * VAT3( uPW, iip1,jj,kk)
01861      - VAT3( uSW, ip1,jp1,km1) * VAT3(dPNW, iip1,jj,kk)
01862      - VAT3( oNE, i,j,k) * VAT3(oPNW, iip1,jj,kk)
01863      - VAT3( uNE, i,j,k) * VAT3(uPNW, iip1,jj,kk));
01864
01865      TMP3_XOE =
01866      - VAT3( uPC, ii,jj,kk) * ( - VAT3( uNW, ip1,jm1,k) * VAT3(oPSW, iip1,jj,kk)
01867      - VAT3( oNW, ip1,jm1,kp1) * VAT3(uPSW, iip1,jj,kk)
01868      - VAT3( uW, ip1,j,k) * VAT3( oPW, iip1,jj,kk)
01869      - VAT3( oE, i,j,kp1) * VAT3( uPW, iip1,jj,kk)
01870      - VAT3( uSW, ip1,jp1,k) * VAT3(oPNW, iip1,jj,kk)
01871      - VAT3( oNE, i,j,kp1) * VAT3(uPNW, iip1,jj,kk))
01872
01873      - VAT3( dPN, ii,jj,kk) * ( - VAT3( oNW, ip1,j,km1) * VAT3( dPW, iip1,jj,kk)
01874      - VAT3( uSE, i,jp1,km1) * VAT3( oPW, iip1,jj,kk)
01875      - VAT3( oE, i,jp1,km1) * VAT3(dPNW, iip1,jj,kk)
01876      - VAT3( uE, i,jp1,km1) * VAT3(oPNW, iip1,jj,kk))
01877
01878      - VAT3( oPN, ii,jj,kk) * ( - VAT3( uNW, ip1,j,km1) * VAT3( dPW, iip1,jj,kk)
01879      - VAT3( oNW, ip1,j,k) * VAT3( oPW, iip1,jj,kk)
01880      - VAT3( uSE, i,jp1,k) * VAT3( uPW, iip1,jj,kk)
01881      - VAT3( uW, ip1,jp1,km1) * VAT3(dPNW, iip1,jj,kk)
01882      - VAT3( oE, i,jp1,k) * VAT3(oPNW, iip1,jj,kk)
01883      - VAT3( uE, i,jp1,k) * VAT3(uPNW, iip1,jj,kk));
01884
01885      TMP4_XOE =
01886      - VAT3( uPN, ii,jj,kk) * ( - VAT3( uNW, ip1,j,k) * VAT3( oPW, iip1,jj,kk)
01887      - VAT3( oNW, ip1,j,kp1) * VAT3( uPW, iip1,jj,kk)
01888      - VAT3( uW, ip1,jp1,k) * VAT3(oPNW, iip1,jj,kk)
01889      - VAT3( oE, i,jp1,kp1) * VAT3(uPNW, iip1,jj,kk))
01890
01891      - VAT3(dPSE, ii,jj,kk) * ( VAT3( oC, ip1,jm1,km1) * VAT3(dPSW, iip1,jj,kk)
01892      - VAT3( uC, ip1,jm1,km1) * VAT3(oPSW, iip1,jj,kk)
01893      - VAT3( oN, ip1,jm1,km1) * VAT3( dPW, iip1,jj,kk)
01894      - VAT3( uN, ip1,jm1,km1) * VAT3( oPW, iip1,jj,kk)
01895      - VAT3( oE, ip1,jm1,km1) * VAT3( dPS, iip1,jj,kk)
01896      - VAT3( uE, ip1,jm1,km1) * VAT3( oPS, iip1,jj,kk)

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01897             - VAT3( oNE, ip1,jm1,km1) * VAT3( dPC, iip1,jj,kk)
01898             - VAT3( uNE, ip1,jm1,km1) * VAT3( oPC, iip1,jj,kk));
01899
01900 TMP5_XOE =
01901     - VAT3(oPSE, ii,jj,kk) * (- VAT3( uC, ip1,jm1,km1) * VAT3(dPSW, iip1,jj,kk)
01902       + VAT3( oC, ip1,jm1,k) * VAT3(oPSW, iip1,jj,kk)
01903       - VAT3( uC, ip1,jm1,k) * VAT3(uPSW, iip1,jj,kk)
01904       - VAT3( uS, ip1,j,km1) * VAT3( dPW, iip1,jj,kk)
01905       - VAT3( oN, ip1,jm1,k) * VAT3( oPW, iip1,jj,kk)
01906       - VAT3( uN, ip1,jm1,k) * VAT3( uPW, iip1,jj,kk)
01907       - VAT3( uW, ip2,jm1,km1) * VAT3( dPS, iip1,jj,kk)
01908       - VAT3( oE, ip1,jm1,k) * VAT3( oPS, iip1,jj,kk)
01909       - VAT3( uE, ip1,jm1,k) * VAT3( uPS, iip1,jj,kk)
01910       - VAT3( uSW, ip2,j,km1) * VAT3( dPC, iip1,jj,kk)
01911       - VAT3( oNE, ip1,jm1,k) * VAT3( oPC, iip1,jj,kk)
01912       - VAT3( uNE, ip1,jm1,k) * VAT3( uPC, iip1,jj,kk));
01913
01914 TMP6_XOE =
01915     - VAT3(uPSE, ii,jj,kk) * (- VAT3( uC, ip1,jm1,k) * VAT3(oPSW, iip1,jj,kk)
01916       + VAT3( oC, ip1,jm1,kp1) * VAT3(uPSW, iip1,jj,kk)
01917       - VAT3( uS, ip1,j,k) * VAT3( oPW, iip1,jj,kk)
01918       - VAT3( oN, ip1,jm1,kp1) * VAT3( uPW, iip1,jj,kk)
01919       - VAT3( uW, ip2,jm1,k) * VAT3( oPS, iip1,jj,kk)
01920       - VAT3( oE, ip1,jm1,kp1) * VAT3( uPS, iip1,jj,kk)
01921       - VAT3( uSW, ip2,j,k) * VAT3( oPC, iip1,jj,kk)
01922       - VAT3( oNE, ip1,jm1,kp1) * VAT3( uPC, iip1,jj,kk));
01923
01924 TMP7_XOE =
01925     - VAT3( dPE, ii,jj,kk) * (- VAT3( oN, ip1,jm1,km1) * VAT3(dPSW, iip1,jj,kk)
01926       - VAT3( uS, ip1,j,km1) * VAT3(oPSW, iip1,jj,kk)
01927       + VAT3( oC, ip1,j,km1) * VAT3( dPW, iip1,jj,kk)
01928       - VAT3( uC, ip1,j,km1) * VAT3( oPW, iip1,jj,kk)
01929       - VAT3( oN, ip1,j,km1) * VAT3(dPNW, iip1,jj,kk)
01930       - VAT3( uN, ip1,j,km1) * VAT3(oPNW, iip1,jj,kk)
01931       - VAT3( oNW, ip2,jm1,km1) * VAT3( dPS, iip1,jj,kk)
01932       - VAT3( uSE, ip1,j,km1) * VAT3( oPS, iip1,jj,kk)
01933       - VAT3( oE, ip1,j,km1) * VAT3( dPC, iip1,jj,kk)
01934       - VAT3( uE, ip1,j,km1) * VAT3( oPC, iip1,jj,kk)
01935       - VAT3( oNE, ip1,j,km1) * VAT3( dPN, iip1,jj,kk)
01936       - VAT3( uNE, ip1,j,km1) * VAT3( oPN, iip1,jj,kk));
01937
01938 TMP8_XOE =
01939     - VAT3( oPE, ii,jj,kk) * (- VAT3( uN, ip1,jm1,km1) * VAT3(dPSW, iip1,jj,kk)
01940       - VAT3( oN, ip1,jm1,k) * VAT3(oPSW, iip1,jj,kk)
01941       - VAT3( uS, ip1,j,k) * VAT3(uPSW, iip1,jj,kk)
01942       - VAT3( uC, ip1,j,km1) * VAT3( dPW, iip1,jj,kk)
01943       + VAT3( oC, ip1,j,k) * VAT3( oPW, iip1,jj,kk)
01944       - VAT3( uC, ip1,j,k) * VAT3( uPW, iip1,jj,kk)
01945       - VAT3( uS, ip1,jp1,km1) * VAT3(dPNW, iip1,jj,kk)
01946       - VAT3( oN, ip1,j,k) * VAT3(oPNW, iip1,jj,kk)
01947       - VAT3( uN, ip1,j,k) * VAT3(uPNW, iip1,jj,kk)
01948       - VAT3( uNW, ip2,jm1,km1) * VAT3( dPS, iip1,jj,kk)
01949       - VAT3( oNW, ip2,jm1,k) * VAT3( oPS, iip1,jj,kk)
01950       - VAT3( uSE, ip1,j,k) * VAT3( uPS, iip1,jj,kk)
01951       - VAT3( uW, ip2,j,km1) * VAT3( dPC, iip1,jj,kk)
01952       - VAT3( oE, ip1,j,k) * VAT3( oPC, iip1,jj,kk)
01953       - VAT3( uE, ip1,j,k) * VAT3( uPC, iip1,jj,kk)
01954       - VAT3( uSW, ip2,jp1,km1) * VAT3( dPN, iip1,jj,kk)
01955       - VAT3( oNE, ip1,j,k) * VAT3( oPN, iip1,jj,kk)
01956       - VAT3( uNE, ip1,j,k) * VAT3( uPN, iip1,jj,kk));
01957
01958 TMP9_XOE =
01959     - VAT3( uPE, ii,jj,kk) * (- VAT3( uN, ip1,jm1,k) * VAT3(oPSW, iip1,jj,kk)
01960       - VAT3( oN, ip1,jm1,kp1) * VAT3(uPSW, iip1,jj,kk)
01961       - VAT3( uC, ip1,j,k) * VAT3( oPW, iip1,jj,kk)
01962       + VAT3( oC, ip1,j,kp1) * VAT3( uPW, iip1,jj,kk)
01963       - VAT3( uS, ip1,jp1,k) * VAT3(oPNW, iip1,jj,kk)
01964       - VAT3( oN, ip1,j,kp1) * VAT3(uPNW, iip1,jj,kk)
01965       - VAT3( uNW, ip2,jm1,k) * VAT3( oPS, iip1,jj,kk)
01966       - VAT3( oNW, ip2,jm1,kp1) * VAT3( uPS, iip1,jj,kk)
01967       - VAT3( uW, ip2,j,k) * VAT3( oPC, iip1,jj,kk)
01968       - VAT3( oE, ip1,j,kp1) * VAT3( uPC, iip1,jj,kk)
01969       - VAT3( uSW, ip2,jp1,k) * VAT3( oPN, iip1,jj,kk)
01970       - VAT3( oNE, ip1,j,kp1) * VAT3( uPN, iip1,jj,kk));
01971
01972 TMP10_XOE =
01973     - VAT3(dPNE, ii,jj,kk) * (- VAT3( oN, ip1,j,km1) * VAT3( dPW, iip1,jj,kk)
01974       - VAT3( uS, ip1,jp1,km1) * VAT3( oPW, iip1,jj,kk)
01975       + VAT3( oC, ip1,jp1,km1) * VAT3(dPNW, iip1,jj,kk)
01976       - VAT3( uC, ip1,jp1,km1) * VAT3(oPNW, iip1,jj,kk)
01977       - VAT3( oNW, ip2,j,km1) * VAT3( dPC, iip1,jj,kk)

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01978             - VAT3( uSE, ip1,jp1,km1) * VAT3( oPC, iip1,jj,kk)
01979             - VAT3( oE, ip1,jp1,km1) * VAT3( dPN, iip1,jj,kk)
01980             - VAT3( uE, ip1,jp1,km1) * VAT3( oPN, iip1,jj,kk));
01981
01982 TMP11_XOE =
01983     - VAT3(oPNE, ii,jj,kk) * ( - VAT3( uN, ip1,j,km1) * VAT3( dPW, iip1,jj,kk)
01984     - VAT3( oN, ip1,j,k) * VAT3( oPW, iip1,jj,kk)
01985     - VAT3( uS, ip1,jp1,k) * VAT3( uPW, iip1,jj,kk)
01986     - VAT3( uC, ip1,jp1,km1) * VAT3( dPNW, iip1,jj,kk)
01987     + VAT3( oC, ip1,jp1,k) * VAT3( oPNW, iip1,jj,kk)
01988     - VAT3( uC, ip1,jp1,k) * VAT3( uPNW, iip1,jj,kk)
01989     - VAT3( uNW, ip2,j,km1) * VAT3( dPC, iip1,jj,kk)
01990     - VAT3( oNW, ip2,j,k) * VAT3( oPC, iip1,jj,kk)
01991     - VAT3( uSE, ip1,jp1,k) * VAT3( uPC, iip1,jj,kk)
01992     - VAT3( uW, ip2,jp1,km1) * VAT3( dPN, iip1,jj,kk)
01993     - VAT3( oE, ip1,jp1,k) * VAT3( oPN, iip1,jj,kk)
01994     - VAT3( uE, ip1,jp1,k) * VAT3( uPN, iip1,jj,kk));
01995
01996 TMP12_XOE =
01997     - VAT3(uPNE, ii,jj,kk) * ( - VAT3( uN, ip1,j,k) * VAT3( oPW, iip1,jj,kk)
01998     - VAT3( oN, ip1,j,kp1) * VAT3( uPW, iip1,jj,kk)
01999     - VAT3( uC, ip1,jp1,k) * VAT3( oPNW, iip1,jj,kk)
02000     + VAT3( oC, ip1,jp1,kp1) * VAT3( uPNW, iip1,jj,kk)
02001     - VAT3( uNW, ip2,j,k) * VAT3( oPC, iip1,jj,kk)
02002     - VAT3( oNW, ip2,j,kp1) * VAT3( uPC, iip1,jj,kk)
02003     - VAT3( uW, ip2,jp1,k) * VAT3( oPN, iip1,jj,kk)
02004     - VAT3( oE, ip1,jp1,kp1) * VAT3( uPN, iip1,jj,kk));
02005
02006 VAT3( XoE, ii,jj,kk) = TMP1_XOE + TMP2_XOE + TMP3_XOE + TMP4_XOE
02007     + TMP5_XOE + TMP6_XOE + TMP7_XOE + TMP8_XOE + TMP9_XOE
02008     + TMP10_XOE + TMP11_XOE + TMP12_XOE;
02009
02010     //fprintf(data, "%19.12E\n", VAT3(XoE, ii, jj, kk));
02011
02012     /* *****
02013     * *** > ON;
02014     * *****/
02015
02016     // VAT3( XoN, ii,jj,kk) =
02017 TMP1_XON =
02018     - VAT3( dPW, ii,jj,kk) * ( - VAT3( oN, im1,j,km1) * VAT3(dPSW, ii,jjp1,kk)
02019     - VAT3( uN, im1,j,km1) * VAT3(oPSW, ii,jjp1,kk)
02020     - VAT3( oNE, im1,j,km1) * VAT3( dPS, ii,jjp1,kk)
02021     - VAT3( uNE, im1,j,km1) * VAT3( oPS, ii,jjp1,kk))
02022
02023     - VAT3( oPW, ii,jj,kk) * ( - VAT3( uS, im1,jp1,km1) * VAT3(dPSW, ii,jjp1,kk)
02024     - VAT3( oN, im1,j,k) * VAT3(oPSW, ii,jjp1,kk)
02025     - VAT3( uN, im1,j,k) * VAT3(uPSW, ii,jjp1,kk)
02026     - VAT3( uSW, i,jp1,km1) * VAT3( dPS, ii,jjp1,kk)
02027     - VAT3( oNE, im1,j,k) * VAT3( oPS, ii,jjp1,kk)
02028     - VAT3( uNE, im1,j,k) * VAT3( uPS, ii,jjp1,kk))
02029
02030     - VAT3( uPW, ii,jj,kk) * ( - VAT3( uS, im1,jp1,k) * VAT3(oPSW, ii,jjp1,kk)
02031     - VAT3( oN, im1,j,kp1) * VAT3(uPSW, ii,jjp1,kk)
02032     - VAT3( uSW, i,jp1,k) * VAT3( oPS, ii,jjp1,kk)
02033     - VAT3( oNE, im1,j,kp1) * VAT3( uPS, ii,jjp1,kk));
02034
02035 TMP2_XON =
02036     - VAT3(dPNW, ii,jj,kk) * ( VAT3( oC, im1,jp1,km1) * VAT3(dPSW, ii,jjp1,kk)
02037     - VAT3( uC, im1,jp1,km1) * VAT3(oPSW, ii,jjp1,kk)
02038     - VAT3( oN, im1,jp1,km1) * VAT3( dPW, ii,jjp1,kk)
02039     - VAT3( uN, im1,jp1,km1) * VAT3( oPW, ii,jjp1,kk)
02040     - VAT3( oE, im1,jp1,km1) * VAT3( dPS, ii,jjp1,kk)
02041     - VAT3( uE, im1,jp1,km1) * VAT3( oPS, ii,jjp1,kk)
02042     - VAT3( oNE, im1,jp1,km1) * VAT3( dPC, ii,jjp1,kk)
02043     - VAT3( uNE, im1,jp1,km1) * VAT3( oPC, ii,jjp1,kk));
02044
02045 TMP3_XON =
02046     - VAT3(oPNW, ii,jj,kk) * ( - VAT3( uC, im1,jp1,km1) * VAT3(dPSW, ii,jjp1,kk)
02047     + VAT3( oC, im1,jp1,k) * VAT3(oPSW, ii,jjp1,kk)
02048     - VAT3( uC, im1,jp1,k) * VAT3(uPSW, ii,jjp1,kk)
02049     - VAT3( uS, im1,jp2,km1) * VAT3( dPW, ii,jjp1,kk)
02050     - VAT3( oN, im1,jp1,k) * VAT3( oPW, ii,jjp1,kk)
02051     - VAT3( uN, im1,jp1,k) * VAT3( uPW, ii,jjp1,kk)
02052     - VAT3( uW, i,jp1,km1) * VAT3( dPS, ii,jjp1,kk)
02053     - VAT3( oE, im1,jp1,k) * VAT3( oPS, ii,jjp1,kk)
02054     - VAT3( uE, im1,jp1,k) * VAT3( uPS, ii,jjp1,kk)
02055     - VAT3( uSW, i,jp2,km1) * VAT3( dPC, ii,jjp1,kk)
02056     - VAT3( oNE, im1,jp1,k) * VAT3( oPC, ii,jjp1,kk)
02057     - VAT3( uNE, im1,jp1,k) * VAT3( uPC, ii,jjp1,kk));
02058

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02059     TMP4_XON =
02060     - VAT3( uPNW, ii,jj,kk) * ( - VAT3( uC, im1,jp1,k) * VAT3( oPSW, ii,jjp1,kk)
02061       + VAT3( oC, im1,jp1,kp1) * VAT3( uPSW, ii,jjp1,kk)
02062       - VAT3( uS, im1,jp2,k) * VAT3( oPW, ii,jjp1,kk)
02063       - VAT3( oN, im1,jp1,kp1) * VAT3( uPW, ii,jjp1,kk)
02064       - VAT3( uW, i,jp1,k) * VAT3( oPS, ii,jjp1,kk)
02065       - VAT3( oE, im1,jp1,kp1) * VAT3( uPS, ii,jjp1,kk)
02066       - VAT3( uSW, i,jp2,k) * VAT3( oPC, ii,jjp1,kk)
02067       - VAT3( oNE, im1,jp1,kp1) * VAT3( uPC, ii,jjp1,kk))
02068
02069     - VAT3( dPC, ii,jj,kk) * ( - VAT3( oNW, i,j,kml) * VAT3( dPSW, ii,jjp1,kk)
02070       - VAT3( uNW, i,j,kml) * VAT3( oPSW, ii,jjp1,kk)
02071       - VAT3( oN, i,j,kml) * VAT3( dPS, ii,jjp1,kk)
02072       - VAT3( uN, i,j,kml) * VAT3( oPS, ii,jjp1,kk)
02073       - VAT3( oNE, i,j,kml) * VAT3( dPSE, ii,jjp1,kk)
02074       - VAT3( uNE, i,j,kml) * VAT3( oPSE, ii,jjp1,kk));
02075
02076     TMP5_XON =
02077     - VAT3( oPC, ii,jj,kk) * ( - VAT3( uSE, im1,jp1,kml) * VAT3( dPSW, ii,jjp1,kk)
02078       - VAT3( oNW, i,j,k) * VAT3( oPSW, ii,jjp1,kk)
02079       - VAT3( uNW, i,j,k) * VAT3( uPSW, ii,jjp1,kk)
02080       - VAT3( uS, i,jp1,kml) * VAT3( dPS, ii,jjp1,kk)
02081       - VAT3( oN, i,j,k) * VAT3( oPS, ii,jjp1,kk)
02082       - VAT3( uN, i,j,k) * VAT3( uPS, ii,jjp1,kk)
02083       - VAT3( uSW, ip1,jp1,kml) * VAT3( dPSE, ii,jjp1,kk)
02084       - VAT3( oNE, i,j,k) * VAT3( oPSE, ii,jjp1,kk)
02085       - VAT3( uNE, i,j,k) * VAT3( uPSE, ii,jjp1,kk))
02086
02087     - VAT3( uPC, ii,jj,kk) * ( - VAT3( uSE, im1,jp1,k) * VAT3( oPSW, ii,jjp1,kk)
02088       - VAT3( oNW, i,j,kp1) * VAT3( uPSW, ii,jjp1,kk)
02089       - VAT3( uS, i,jp1,k) * VAT3( oPS, ii,jjp1,kk)
02090       - VAT3( oN, i,j,kp1) * VAT3( uPS, ii,jjp1,kk)
02091       - VAT3( uSW, ip1,jp1,k) * VAT3( oPSE, ii,jjp1,kk)
02092       - VAT3( oNE, i,j,kp1) * VAT3( uPSE, ii,jjp1,kk));
02093
02094     TMP6_XON =
02095     - VAT3( dPN, ii,jj,kk) * ( - VAT3( oE, im1,jp1,kml) * VAT3( dPSW, ii,jjp1,kk)
02096       - VAT3( uW, i,jp1,kml) * VAT3( oPSW, ii,jjp1,kk)
02097       - VAT3( oNW, i,jp1,kml) * VAT3( dPW, ii,jjp1,kk)
02098       - VAT3( uNW, i,jp1,kml) * VAT3( oPW, ii,jjp1,kk)
02099       + VAT3( oC, i,jp1,kml) * VAT3( dPS, ii,jjp1,kk)
02100       - VAT3( uC, i,jp1,kml) * VAT3( oPS, ii,jjp1,kk)
02101       - VAT3( oN, i,jp1,kml) * VAT3( dPC, ii,jjp1,kk)
02102       - VAT3( uN, i,jp1,kml) * VAT3( oPC, ii,jjp1,kk)
02103       - VAT3( oE, i,jp1,kml) * VAT3( dPSE, ii,jjp1,kk)
02104       - VAT3( uE, i,jp1,kml) * VAT3( oPSE, ii,jjp1,kk)
02105       - VAT3( oNE, i,jp1,kml) * VAT3( dPE, ii,jjp1,kk)
02106       - VAT3( uNE, i,jp1,kml) * VAT3( oPE, ii,jjp1,kk));
02107
02108     TMP7_XON =
02109     - VAT3( oPN, ii,jj,kk) * ( - VAT3( uE, im1,jp1,kml) * VAT3( dPSW, ii,jjp1,kk)
02110       - VAT3( oE, im1,jp1,k) * VAT3( oPSW, ii,jjp1,kk)
02111       - VAT3( uW, i,jp1,k) * VAT3( uPSW, ii,jjp1,kk)
02112       - VAT3( uSE, im1,jp2,kml) * VAT3( dPW, ii,jjp1,kk)
02113       - VAT3( oNW, i,jp1,k) * VAT3( oPW, ii,jjp1,kk)
02114       - VAT3( uNW, i,jp1,k) * VAT3( uPW, ii,jjp1,kk)
02115       - VAT3( uC, i,jp1,kml) * VAT3( dPS, ii,jjp1,kk)
02116       + VAT3( oC, i,jp1,k) * VAT3( oPS, ii,jjp1,kk)
02117       - VAT3( uC, i,jp1,k) * VAT3( uPS, ii,jjp1,kk)
02118       - VAT3( uS, i,jp2,kml) * VAT3( dPC, ii,jjp1,kk)
02119       - VAT3( oN, i,jp1,k) * VAT3( oPC, ii,jjp1,kk)
02120       - VAT3( uN, i,jp1,k) * VAT3( uPC, ii,jjp1,kk)
02121       - VAT3( uW, ip1,jp1,kml) * VAT3( dPSE, ii,jjp1,kk)
02122       - VAT3( oE, i,jp1,k) * VAT3( oPSE, ii,jjp1,kk)
02123       - VAT3( uE, i,jp1,k) * VAT3( uPSE, ii,jjp1,kk)
02124       - VAT3( uSW, ip1,jp2,kml) * VAT3( dPE, ii,jjp1,kk)
02125       - VAT3( oNE, i,jp1,k) * VAT3( oPE, ii,jjp1,kk)
02126       - VAT3( uNE, i,jp1,k) * VAT3( uPE, ii,jjp1,kk));
02127
02128     TMP8_XON =
02129     - VAT3( uPN, ii,jj,kk) * ( - VAT3( uE, im1,jp1,k) * VAT3( oPSW, ii,jjp1,kk)
02130       - VAT3( oE, im1,jp1,kp1) * VAT3( uPSW, ii,jjp1,kk)
02131       - VAT3( uSE, im1,jp2,k) * VAT3( oPW, ii,jjp1,kk)
02132       - VAT3( oNW, i,jp1,kp1) * VAT3( uPW, ii,jjp1,kk)
02133       - VAT3( uC, i,jp1,k) * VAT3( oPS, ii,jjp1,kk)
02134       + VAT3( oC, i,jp1,kp1) * VAT3( uPS, ii,jjp1,kk)
02135       - VAT3( uS, i,jp2,k) * VAT3( oPC, ii,jjp1,kk)
02136       - VAT3( oN, i,jp1,kp1) * VAT3( uPC, ii,jjp1,kk)
02137       - VAT3( uW, ip1,jp1,k) * VAT3( oPSE, ii,jjp1,kk)
02138       - VAT3( oE, i,jp1,kp1) * VAT3( uPSE, ii,jjp1,kk)
02139       - VAT3( uSW, ip1,jp2,k) * VAT3( oPE, ii,jjp1,kk)

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02140             - VAT3( oNE, i, jpl, kpl) * VAT3( uPE, ii, jjpl, kk))
02141
02142     - VAT3( dPE, ii, jj, kk) * (- VAT3( oNW, ip1, j, kml) * VAT3( dPS, ii, jjpl, kk)
02143       - VAT3( uNW, ip1, j, kml) * VAT3( oPS, ii, jjpl, kk)
02144       - VAT3( oN, ip1, j, kml) * VAT3( dPSE, ii, jjpl, kk)
02145       - VAT3( uN, ip1, j, kml) * VAT3( oPSE, ii, jjpl, kk));
02146
02147     TMP9_XON =
02148     - VAT3( oPE, ii, jj, kk) * (- VAT3( uSE, i, jpl, kml) * VAT3( dPS, ii, jjpl, kk)
02149       - VAT3( oNW, ip1, j, k) * VAT3( oPS, ii, jjpl, kk)
02150       - VAT3( uNW, ip1, j, k) * VAT3( uPS, ii, jjpl, kk)
02151       - VAT3( uS, ip1, jpl, kml) * VAT3( dPSE, ii, jjpl, kk)
02152       - VAT3( oN, ip1, j, k) * VAT3( oPSE, ii, jjpl, kk)
02153       - VAT3( uN, ip1, j, k) * VAT3( uPSE, ii, jjpl, kk))
02154
02155     - VAT3( uPE, ii, jj, kk) * (- VAT3( uSE, i, jpl, k) * VAT3( oPS, ii, jjpl, kk)
02156       - VAT3( oNW, ip1, j, kpl) * VAT3( uPS, ii, jjpl, kk)
02157       - VAT3( uS, ip1, jpl, k) * VAT3( oPSE, ii, jjpl, kk)
02158       - VAT3( oN, ip1, j, kpl) * VAT3( uPSE, ii, jjpl, kk));
02159
02160     TMP10_XON =
02161     - VAT3( dPNE, ii, jj, kk) * (- VAT3( oE, i, jpl, kml) * VAT3( dPS, ii, jjpl, kk)
02162       - VAT3( uW, ip1, jpl, kml) * VAT3( oPS, ii, jjpl, kk)
02163       - VAT3( oNW, ip1, jpl, kml) * VAT3( dPC, ii, jjpl, kk)
02164       - VAT3( uNW, ip1, jpl, kml) * VAT3( oPC, ii, jjpl, kk)
02165       + VAT3( oC, ip1, jpl, kml) * VAT3( dPSE, ii, jjpl, kk)
02166       - VAT3( uC, ip1, jpl, kml) * VAT3( oPSE, ii, jjpl, kk)
02167       - VAT3( oN, ip1, jpl, kml) * VAT3( dPE, ii, jjpl, kk)
02168       - VAT3( uN, ip1, jpl, kml) * VAT3( oPE, ii, jjpl, kk));
02169
02170     TMP11_XON =
02171     - VAT3( oPNE, ii, jj, kk) * (- VAT3( uE, i, jpl, kml) * VAT3( dPS, ii, jjpl, kk)
02172       - VAT3( oE, i, jpl, k) * VAT3( oPS, ii, jjpl, kk)
02173       - VAT3( uW, ip1, jpl, k) * VAT3( uPS, ii, jjpl, kk)
02174       - VAT3( uSE, i, jp2, kml) * VAT3( dPC, ii, jjpl, kk)
02175       - VAT3( oNW, ip1, jpl, k) * VAT3( oPC, ii, jjpl, kk)
02176       - VAT3( uNW, ip1, jpl, k) * VAT3( uPC, ii, jjpl, kk)
02177       - VAT3( uC, ip1, jpl, kml) * VAT3( dPSE, ii, jjpl, kk)
02178       + VAT3( oC, ip1, jpl, k) * VAT3( oPSE, ii, jjpl, kk)
02179       - VAT3( uC, ip1, jpl, k) * VAT3( uPSE, ii, jjpl, kk)
02180       - VAT3( uS, ip1, jp2, kml) * VAT3( dPE, ii, jjpl, kk)
02181       - VAT3( oN, ip1, jpl, k) * VAT3( oPE, ii, jjpl, kk)
02182       - VAT3( uN, ip1, jpl, k) * VAT3( uPE, ii, jjpl, kk));
02183
02184     TMP12_XON =
02185     - VAT3( uPNE, ii, jj, kk) * (- VAT3( uE, i, jpl, k) * VAT3( oPS, ii, jjpl, kk)
02186       - VAT3( oE, i, jpl, kpl) * VAT3( uPS, ii, jjpl, kk)
02187       - VAT3( uSE, i, jp2, k) * VAT3( oPC, ii, jjpl, kk)
02188       - VAT3( oNW, ip1, jpl, kpl) * VAT3( uPC, ii, jjpl, kk)
02189       - VAT3( uC, ip1, jpl, k) * VAT3( oPSE, ii, jjpl, kk)
02190       + VAT3( oC, ip1, jpl, kpl) * VAT3( uPSE, ii, jjpl, kk)
02191       - VAT3( uS, ip1, jp2, k) * VAT3( oPE, ii, jjpl, kk)
02192       - VAT3( oN, ip1, jpl, kpl) * VAT3( uPE, ii, jjpl, kk));
02193
02194     VAT3( XoN, ii, jj, kk) = TMP1_XON + TMP2_XON + TMP3_XON + TMP4_XON
02195     + TMP5_XON + TMP6_XON + TMP7_XON + TMP8_XON + TMP9_XON
02196     + TMP10_XON + TMP11_XON + TMP12_XON;
02197
02198     //fprintf(data, "%19.12E\n", VAT3(XoN, ii, jj, kk));
02199
02200     /* *****
02201      * *** > UC;
02202      * *****
02203
02204     // VAT3( XuC, ii, jj, kk) =
02205     TMP1_XUC =
02206     - VAT3( oPSW, ii, jj, kk) * (- VAT3( uC, iml, jml, k) * VAT3( dPSW, ii, jj, kkpl)
02207       - VAT3( uN, iml, jml, k) * VAT3( dPW, ii, jj, kkpl)
02208       - VAT3( uE, iml, jml, k) * VAT3( dPS, ii, jj, kkpl)
02209       - VAT3( uNE, iml, jml, k) * VAT3( dPC, ii, jj, kkpl))
02210
02211     - VAT3( uPSW, ii, jj, kk) * ( VAT3( oC, iml, jml, kpl) * VAT3( dPSW, ii, jj, kkpl)
02212       - VAT3( uC, iml, jml, kpl) * VAT3( oPSW, ii, jj, kkpl)
02213       - VAT3( oN, iml, jml, kpl) * VAT3( dPW, ii, jj, kkpl)
02214       - VAT3( uN, iml, jml, kpl) * VAT3( oPW, ii, jj, kkpl)
02215       - VAT3( oE, iml, jml, kpl) * VAT3( dPS, ii, jj, kkpl)
02216       - VAT3( uE, iml, jml, kpl) * VAT3( oPS, ii, jj, kkpl)
02217       - VAT3( oNE, iml, jml, kpl) * VAT3( dPC, ii, jj, kkpl)
02218       - VAT3( uNE, iml, jml, kpl) * VAT3( oPC, ii, jj, kkpl));
02219
02220

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02221     TMP2_XUC =
02222     - VAT3( oPW, ii,jj,kk) * (- VAT3( uS, iml,j,k) * VAT3(dPSW, ii,jj,kkp1)
02223       - VAT3( uC, iml,j,k) * VAT3( dPW, ii,jj,kkp1)
02224       - VAT3( uN, iml,j,k) * VAT3(dPNW, ii,jj,kkp1)
02225       - VAT3( uSE, iml,j,k) * VAT3( dPS, ii,jj,kkp1)
02226       - VAT3( uE, iml,j,k) * VAT3( dPC, ii,jj,kkp1)
02227       - VAT3( uNE, iml,j,k) * VAT3( dPN, ii,jj,kkp1));
02228
02229     TMP3_XUC =
02230     - VAT3( uPW, ii,jj,kk) * (- VAT3( oN, iml,jml,kp1) * VAT3(dPSW, ii,jj,kkp1)
02231       - VAT3( uS, iml,j,kp1) * VAT3(oPSW, ii,jj,kkp1)
02232       + VAT3( oC, iml,j,kp1) * VAT3( dPW, ii,jj,kkp1)
02233       - VAT3( uC, iml,j,kp1) * VAT3( oPW, ii,jj,kkp1)
02234       - VAT3( oN, iml,j,kp1) * VAT3(dPNW, ii,jj,kkp1)
02235       - VAT3( uN, iml,j,kp1) * VAT3(oPNW, ii,jj,kkp1)
02236       - VAT3( oNW, i,jml,kp1) * VAT3( dPS, ii,jj,kkp1)
02237       - VAT3( uSE, iml,j,kp1) * VAT3( oPS, ii,jj,kkp1)
02238       - VAT3( oE, iml,j,kp1) * VAT3( dPC, ii,jj,kkp1)
02239       - VAT3( uE, iml,j,kp1) * VAT3( oPC, ii,jj,kkp1)
02240       - VAT3( oNE, iml,j,kp1) * VAT3( dPN, ii,jj,kkp1)
02241       - VAT3( uNE, iml,j,kp1) * VAT3( oPN, ii,jj,kkp1))
02242
02243     - VAT3(oPNW, ii,jj,kk) * (- VAT3( uS, iml,jp1,k) * VAT3( dPW, ii,jj,kkp1)
02244       - VAT3( uC, iml,jp1,k) * VAT3(dPNW, ii,jj,kkp1)
02245       - VAT3( uSE, iml,jp1,k) * VAT3( dPC, ii,jj,kkp1)
02246       - VAT3( uE, iml,jp1,k) * VAT3( dPN, ii,jj,kkp1));
02247
02248     TMP4_XUC =
02249     - VAT3(uPNW, ii,jj,kk) * (- VAT3( oN, iml,j,kp1) * VAT3( dPW, ii,jj,kkp1)
02250       - VAT3( uS, iml,jp1,kp1) * VAT3( oPW, ii,jj,kkp1)
02251       + VAT3( oC, iml,jp1,kp1) * VAT3(dPNW, ii,jj,kkp1)
02252       - VAT3( uC, iml,jp1,kp1) * VAT3(oPNW, ii,jj,kkp1)
02253       - VAT3( oNW, i,j,kp1) * VAT3( dPC, ii,jj,kkp1)
02254       - VAT3( uSE, iml,jp1,kp1) * VAT3( oPC, ii,jj,kkp1)
02255       - VAT3( oE, iml,jp1,kp1) * VAT3( dPN, ii,jj,kkp1)
02256       - VAT3( uE, iml,jp1,kp1) * VAT3( oPN, ii,jj,kkp1))
02257
02258     - VAT3( oPS, ii,jj,kk) * (- VAT3( uW, i,jml,k) * VAT3(dPSW, ii,jj,kkp1)
02259       - VAT3( uNW, i,jml,k) * VAT3( dPW, ii,jj,kkp1)
02260       - VAT3( uC, i,jml,k) * VAT3( dPS, ii,jj,kkp1)
02261       - VAT3( uN, i,jml,k) * VAT3( dPC, ii,jj,kkp1)
02262       - VAT3( uE, i,jml,k) * VAT3(dPSE, ii,jj,kkp1)
02263       - VAT3( uNE, i,jml,k) * VAT3( dPE, ii,jj,kkp1));
02264
02265     TMP5_XUC =
02266     - VAT3( uPS, ii,jj,kk) * (- VAT3( oE, iml,jml,kp1) * VAT3(dPSW, ii,jj,kkp1)
02267       - VAT3( uW, i,jml,kp1) * VAT3(oPSW, ii,jj,kkp1)
02268       - VAT3( oNW, i,jml,kp1) * VAT3( dPW, ii,jj,kkp1)
02269       - VAT3( uNW, i,jml,kp1) * VAT3( oPW, ii,jj,kkp1)
02270       + VAT3( oC, i,jml,kp1) * VAT3( dPS, ii,jj,kkp1)
02271       - VAT3( uC, i,jml,kp1) * VAT3( oPS, ii,jj,kkp1)
02272       - VAT3( oN, i,jml,kp1) * VAT3( dPC, ii,jj,kkp1)
02273       - VAT3( uN, i,jml,kp1) * VAT3( oPC, ii,jj,kkp1)
02274       - VAT3( oE, i,jml,kp1) * VAT3(dPSE, ii,jj,kkp1)
02275       - VAT3( uE, i,jml,kp1) * VAT3(oPSE, ii,jj,kkp1)
02276       - VAT3( oNE, i,jml,kp1) * VAT3( dPE, ii,jj,kkp1)
02277       - VAT3( uNE, i,jml,kp1) * VAT3( oPE, ii,jj,kkp1));
02278
02279     TMP6_XUC =
02280     - VAT3( oPC, ii,jj,kk) * (- VAT3( uSW, i,j,k) * VAT3(dPSW, ii,jj,kkp1)
02281       - VAT3( uW, i,j,k) * VAT3( dPW, ii,jj,kkp1)
02282       - VAT3( uNW, i,j,k) * VAT3(dPNW, ii,jj,kkp1)
02283       - VAT3( uS, i,j,k) * VAT3( dPS, ii,jj,kkp1)
02284       - VAT3( uC, i,j,k) * VAT3( dPC, ii,jj,kkp1)
02285       - VAT3( uN, i,j,k) * VAT3( dPN, ii,jj,kkp1)
02286       - VAT3( uSE, i,j,k) * VAT3(dPSE, ii,jj,kkp1)
02287       - VAT3( uE, i,j,k) * VAT3( dPE, ii,jj,kkp1)
02288       - VAT3( uNE, i,j,k) * VAT3(dPNE, ii,jj,kkp1));
02289
02290     TMP7_XUC =
02291     - VAT3( uPC, ii,jj,kk) * (- VAT3( oNE, iml,jml,kp1) * VAT3(dPSW, ii,jj,kkp1)
02292       - VAT3( uSW, i,j,kp1) * VAT3(oPSW, ii,jj,kkp1)
02293       - VAT3( oE, iml,j,kp1) * VAT3( dPW, ii,jj,kkp1)
02294       - VAT3( uW, i,j,kp1) * VAT3( oPW, ii,jj,kkp1)
02295       - VAT3( oNW, i,j,kp1) * VAT3(dPNW, ii,jj,kkp1)
02296       - VAT3( uNW, i,j,kp1) * VAT3(oPNW, ii,jj,kkp1)
02297       - VAT3( oN, i,jml,kp1) * VAT3( dPS, ii,jj,kkp1)
02298       - VAT3( uS, i,j,kp1) * VAT3( oPS, ii,jj,kkp1)
02299       + VAT3( oC, i,j,kp1) * VAT3( dPC, ii,jj,kkp1)
02300       - VAT3( uC, i,j,kp1) * VAT3( oPC, ii,jj,kkp1)
02301       - VAT3( oN, i,j,kp1) * VAT3( dPN, ii,jj,kkp1)

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02302             - VAT3( uN, i, j, kp1) * VAT3( oPN, ii, jj, kkp1)
02303             - VAT3( oNW, ip1, jml, kp1) * VAT3( dPSE, ii, jj, kkp1)
02304             - VAT3( uSE, i, j, kp1) * VAT3( oPSE, ii, jj, kkp1)
02305             - VAT3( oE, i, j, kp1) * VAT3( dPE, ii, jj, kkp1)
02306             - VAT3( uE, i, j, kp1) * VAT3( oPE, ii, jj, kkp1)
02307             - VAT3( oNE, i, j, kp1) * VAT3( dPNE, ii, jj, kkp1)
02308             - VAT3( uNE, i, j, kp1) * VAT3( oPNE, ii, jj, kkp1));
02309
02310 TMP8_XUC =
02311     - VAT3( oPN, ii, jj, kk) * (- VAT3( uSW, i, jp1, k) * VAT3( dPW, ii, jj, kkp1)
02312     - VAT3( uW, i, jp1, k) * VAT3( dPNW, ii, jj, kkp1)
02313     - VAT3( uS, i, jp1, k) * VAT3( dPC, ii, jj, kkp1)
02314     - VAT3( uC, i, jp1, k) * VAT3( dPN, ii, jj, kkp1)
02315     - VAT3( uSE, i, jp1, k) * VAT3( dPE, ii, jj, kkp1)
02316     - VAT3( uE, i, jp1, k) * VAT3( dPNE, ii, jj, kkp1));
02317
02318 TMP9_XUC =
02319     - VAT3( uPN, ii, jj, kk) * (- VAT3( oNE, im1, j, kp1) * VAT3( dPW, ii, jj, kkp1)
02320     - VAT3( uSW, i, jp1, kp1) * VAT3( oPW, ii, jj, kkp1)
02321     - VAT3( oE, im1, jp1, kp1) * VAT3( dPNW, ii, jj, kkp1)
02322     - VAT3( uW, i, jp1, kp1) * VAT3( oPNW, ii, jj, kkp1)
02323     - VAT3( oN, i, j, kp1) * VAT3( dPC, ii, jj, kkp1)
02324     - VAT3( uS, i, jp1, kp1) * VAT3( oPC, ii, jj, kkp1)
02325     + VAT3( oC, i, jp1, kp1) * VAT3( dPN, ii, jj, kkp1)
02326     - VAT3( uC, i, jp1, kp1) * VAT3( oPN, ii, jj, kkp1)
02327     - VAT3( oNW, ip1, j, kp1) * VAT3( dPE, ii, jj, kkp1)
02328     - VAT3( uSE, i, jp1, kp1) * VAT3( oPE, ii, jj, kkp1)
02329     - VAT3( oE, i, jp1, kp1) * VAT3( dPNE, ii, jj, kkp1)
02330     - VAT3( uE, i, jp1, kp1) * VAT3( oPNE, ii, jj, kkp1) )
02331
02332     - VAT3( oPSE, ii, jj, kk) * (- VAT3( uW, ip1, jml, k) * VAT3( dPS, ii, jj, kkp1)
02333     - VAT3( uNW, ip1, jml, k) * VAT3( dPC, ii, jj, kkp1)
02334     - VAT3( uC, ip1, jml, k) * VAT3( dPSE, ii, jj, kkp1)
02335     - VAT3( uN, ip1, jml, k) * VAT3( dPE, ii, jj, kkp1));
02336
02337 TMP10_XUC =
02338     - VAT3( uPSE, ii, jj, kk) * (- VAT3( oE, i, jml, kp1) * VAT3( dPS, ii, jj, kkp1)
02339     - VAT3( uW, ip1, jml, kp1) * VAT3( oPS, ii, jj, kkp1)
02340     - VAT3( oNW, ip1, jml, kp1) * VAT3( dPC, ii, jj, kkp1)
02341     - VAT3( uNW, ip1, jml, kp1) * VAT3( oPC, ii, jj, kkp1)
02342     + VAT3( oC, ip1, jml, kp1) * VAT3( dPSE, ii, jj, kkp1)
02343     - VAT3( uC, ip1, jml, kp1) * VAT3( oPSE, ii, jj, kkp1)
02344     - VAT3( oN, ip1, jml, kp1) * VAT3( dPE, ii, jj, kkp1)
02345     - VAT3( uN, ip1, jml, kp1) * VAT3( oPE, ii, jj, kkp1) )
02346
02347     - VAT3( oPE, ii, jj, kk) * (- VAT3( uSW, ip1, j, k) * VAT3( dPS, ii, jj, kkp1)
02348     - VAT3( uW, ip1, j, k) * VAT3( dPC, ii, jj, kkp1)
02349     - VAT3( uNW, ip1, j, k) * VAT3( dPN, ii, jj, kkp1)
02350     - VAT3( uS, ip1, j, k) * VAT3( dPSE, ii, jj, kkp1)
02351     - VAT3( uC, ip1, j, k) * VAT3( dPE, ii, jj, kkp1)
02352     - VAT3( uN, ip1, j, k) * VAT3( dPNE, ii, jj, kkp1));
02353
02354 TMP11_XUC =
02355     - VAT3( uPE, ii, jj, kk) * (- VAT3( oNE, i, jml, kp1) * VAT3( dPS, ii, jj, kkp1)
02356     - VAT3( uSW, ip1, j, kp1) * VAT3( oPS, ii, jj, kkp1)
02357     - VAT3( oE, i, j, kp1) * VAT3( dPC, ii, jj, kkp1)
02358     - VAT3( uW, ip1, j, kp1) * VAT3( oPC, ii, jj, kkp1)
02359     - VAT3( oNW, ip1, j, kp1) * VAT3( dPN, ii, jj, kkp1)
02360     - VAT3( uNW, ip1, j, kp1) * VAT3( oPN, ii, jj, kkp1)
02361     - VAT3( oN, ip1, jml, kp1) * VAT3( dPSE, ii, jj, kkp1)
02362     - VAT3( uS, ip1, j, kp1) * VAT3( oPSE, ii, jj, kkp1)
02363     + VAT3( oC, ip1, j, kp1) * VAT3( dPE, ii, jj, kkp1)
02364     - VAT3( uC, ip1, j, kp1) * VAT3( oPE, ii, jj, kkp1)
02365     - VAT3( oN, ip1, j, kp1) * VAT3( dPNE, ii, jj, kkp1)
02366     - VAT3( uN, ip1, j, kp1) * VAT3( oPNE, ii, jj, kkp1));
02367
02368 TMP12_XUC =
02369     - VAT3( oPNE, ii, jj, kk) * (- VAT3( uSW, ip1, jp1, k) * VAT3( dPC, ii, jj, kkp1)
02370     - VAT3( uW, ip1, jp1, k) * VAT3( dPN, ii, jj, kkp1)
02371     - VAT3( uS, ip1, jp1, k) * VAT3( dPE, ii, jj, kkp1)
02372     - VAT3( uC, ip1, jp1, k) * VAT3( dPNE, ii, jj, kkp1) )
02373
02374     - VAT3( uPNE, ii, jj, kk) * (- VAT3( oNE, i, j, kp1) * VAT3( dPC, ii, jj, kkp1)
02375     - VAT3( uSW, ip1, jp1, kp1) * VAT3( oPC, ii, jj, kkp1)
02376     - VAT3( oE, i, jp1, kp1) * VAT3( dPN, ii, jj, kkp1)
02377     - VAT3( uW, ip1, jp1, kp1) * VAT3( oPN, ii, jj, kkp1)
02378     - VAT3( oN, ip1, j, kp1) * VAT3( dPE, ii, jj, kkp1)
02379     - VAT3( uS, ip1, jp1, kp1) * VAT3( oPE, ii, jj, kkp1)
02380     + VAT3( oC, ip1, jp1, kp1) * VAT3( dPNE, ii, jj, kkp1)
02381     - VAT3( uC, ip1, jp1, kp1) * VAT3( oPNE, ii, jj, kkp1));
02382

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02383 VAT3( XuC, ii,jj,kk) = TMP1_XUC + TMP2_XUC + TMP3_XUC + TMP4_XUC
02384 + TMP5_XUC + TMP6_XUC + TMP7_XUC + TMP8_XUC + TMP9_XUC
02385 + TMP10_XUC + TMP11_XUC + TMP12_XUC;
02386
02387 //fprintf(data, "%19.12E\n", VAT3(XuC, ii, jj, kk));
02388
02389 /* *****
02390 * *** > ONE;
02391 * *****
02392
02393 // VAT3(XoNE, ii,jj,kk) =
02394 TMP1_XONE =
02395 - VAT3( dPC, ii,jj,kk) * (- VAT3( oNE, i,j,kml) * VAT3(dPSW, iip1,jjp1,kk)
02396 - VAT3( uNE, i,j,kml) * VAT3(oPSW, iip1,jjp1,kk))
02397
02398 - VAT3( oPC, ii,jj,kk) * (- VAT3( uSW, ip1,jp1,kml) * VAT3(dPSW, iip1,jjp1,kk)
02399 - VAT3( oNE, i,j,k) * VAT3(oPSW, iip1,jjp1,kk)
02400 - VAT3( uNE, i,j,k) * VAT3(uPSW, iip1,jjp1,kk))
02401
02402 - VAT3( uPC, ii,jj,kk) * (- VAT3( uSW, ip1,jp1,k) * VAT3(oPSW, iip1,jjp1,kk)
02403 - VAT3( oNE, i,j,kpl) * VAT3(uPSW, iip1,jjp1,kk))
02404
02405 - VAT3( dPN, ii,jj,kk) * (- VAT3( oE, i,jp1,kml) * VAT3(dPSW, iip1,jjp1,kk)
02406 - VAT3( uE, i,jp1,kml) * VAT3(oPSW, iip1,jjp1,kk)
02407 - VAT3( oNE, i,jp1,kml) * VAT3( dPW, iip1,jjp1,kk)
02408 - VAT3( uNE, i,jp1,kml) * VAT3( oPW, iip1,jjp1,kk));
02409
02410 TMP2_XONE =
02411 - VAT3( oPN, ii,jj,kk) * (- VAT3( uW, ip1,jp1,kml) * VAT3(dPSW, iip1,jjp1,kk)
02412 - VAT3( oE, i,jp1,k) * VAT3(oPSW, iip1,jjp1,kk)
02413 - VAT3( uE, i,jp1,k) * VAT3(uPSW, iip1,jjp1,kk)
02414 - VAT3( uSW, ip1,jp2,kml) * VAT3( dPW, iip1,jjp1,kk)
02415 - VAT3( oNE, i,jp1,k) * VAT3( oPW, iip1,jjp1,kk)
02416 - VAT3( uNE, i,jp1,k) * VAT3( uPW, iip1,jjp1,kk))
02417
02418 - VAT3( uPN, ii,jj,kk) * (- VAT3( uW, ip1,jp1,k) * VAT3(oPSW, iip1,jjp1,kk)
02419 - VAT3( oE, i,jp1,kpl) * VAT3(uPSW, iip1,jjp1,kk)
02420 - VAT3( uSW, ip1,jp2,k) * VAT3( oPW, iip1,jjp1,kk)
02421 - VAT3( oNE, i,jp1,kpl) * VAT3( uPW, iip1,jjp1,kk))
02422
02423 - VAT3( dPE, ii,jj,kk) * (- VAT3( oN, ip1,j,kml) * VAT3(dPSW, iip1,jjp1,kk)
02424 - VAT3( uN, ip1,j,kml) * VAT3(oPSW, iip1,jjp1,kk)
02425 - VAT3( oNE, ip1,j,kml) * VAT3( dPS, iip1,jjp1,kk)
02426 - VAT3( uNE, ip1,j,kml) * VAT3( oPS, iip1,jjp1,kk));
02427
02428 TMP3_XONE =
02429 - VAT3( oPE, ii,jj,kk) * (- VAT3( uS, ip1,jp1,kml) * VAT3(dPSW, iip1,jjp1,kk)
02430 - VAT3( oN, ip1,j,k) * VAT3(oPSW, iip1,jjp1,kk)
02431 - VAT3( uN, ip1,j,k) * VAT3(uPSW, iip1,jjp1,kk)
02432 - VAT3( uSW, ip2,jp1,kml) * VAT3( dPS, iip1,jjp1,kk)
02433 - VAT3( oNE, ip1,j,k) * VAT3( oPS, iip1,jjp1,kk)
02434 - VAT3( uNE, ip1,j,k) * VAT3( uPS, iip1,jjp1,kk))
02435
02436 - VAT3( uPE, ii,jj,kk) * (- VAT3( uS, ip1,jp1,k) * VAT3(oPSW, iip1,jjp1,kk)
02437 - VAT3( oN, ip1,j,kpl) * VAT3(uPSW, iip1,jjp1,kk)
02438 - VAT3( uSW, ip2,jp1,k) * VAT3( oPS, iip1,jjp1,kk)
02439 - VAT3( oNE, ip1,j,kpl) * VAT3( uPS, iip1,jjp1,kk));
02440
02441 TMP4_XONE =
02442 - VAT3(dPNE, ii,jj,kk) * ( VAT3( oC, ip1,jp1,kml) * VAT3(dPSW, iip1,jjp1,kk)
02443 - VAT3( uC, ip1,jp1,kml) * VAT3(oPSW, iip1,jjp1,kk)
02444 - VAT3( oN, ip1,jp1,kml) * VAT3( dPW, iip1,jjp1,kk)
02445 - VAT3( uN, ip1,jp1,kml) * VAT3( oPW, iip1,jjp1,kk)
02446 - VAT3( oE, ip1,jp1,kml) * VAT3( dPS, iip1,jjp1,kk)
02447 - VAT3( uE, ip1,jp1,kml) * VAT3( oPS, iip1,jjp1,kk)
02448 - VAT3( oNE, ip1,jp1,kml) * VAT3( dPC, iip1,jjp1,kk)
02449 - VAT3( uNE, ip1,jp1,kml) * VAT3( oPC, iip1,jjp1,kk));
02450
02451 TMP5_XONE =
02452 - VAT3(oPNE, ii,jj,kk) * (- VAT3( uC, ip1,jp1,kml) * VAT3(dPSW, iip1,jjp1,kk)
02453 + VAT3( oC, ip1,jp1,k) * VAT3(oPSW, iip1,jjp1,kk)
02454 - VAT3( uC, ip1,jp1,k) * VAT3(uPSW, iip1,jjp1,kk)
02455 - VAT3( uS, ip1,jp2,kml) * VAT3( dPW, iip1,jjp1,kk)
02456 - VAT3( oN, ip1,jp1,k) * VAT3( oPW, iip1,jjp1,kk)
02457 - VAT3( uN, ip1,jp1,k) * VAT3( uPW, iip1,jjp1,kk)
02458 - VAT3( uW, ip2,jp1,kml) * VAT3( dPS, iip1,jjp1,kk)
02459 - VAT3( oE, ip1,jp1,k) * VAT3( oPS, iip1,jjp1,kk)
02460 - VAT3( uE, ip1,jp1,k) * VAT3( uPS, iip1,jjp1,kk)
02461 - VAT3( uSW, ip2,jp2,kml) * VAT3( dPC, iip1,jjp1,kk)
02462 - VAT3( oNE, ip1,jp1,k) * VAT3( oPC, iip1,jjp1,kk)
02463 - VAT3( uNE, ip1,jp1,k) * VAT3( uPC, iip1,jjp1,kk));

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02464
02465     TMP6_XONE =
02466         - VAT3(uPNE, ii, jj, kk) * (- VAT3( uC, ip1, jp1, k) * VAT3(oPSW, iip1, jjp1, kk)
02467             + VAT3( oC, ip1, jp1, kp1) * VAT3(uPSW, iip1, jjp1, kk)
02468             - VAT3( uS, ip1, jp2, k) * VAT3( oPW, iip1, jjp1, kk)
02469             - VAT3( oN, ip1, jp1, kp1) * VAT3( uPW, iip1, jjp1, kk)
02470             - VAT3( uW, ip2, jp1, k) * VAT3( oPS, iip1, jjp1, kk)
02471             - VAT3( oE, ip1, jp1, kp1) * VAT3( uPS, iip1, jjp1, kk)
02472             - VAT3( uSW, ip2, jp2, k) * VAT3( oPC, iip1, jjp1, kk)
02473             - VAT3( oNE, ip1, jp1, kp1) * VAT3( uPC, iip1, jjp1, kk));
02474
02475     VAT3(XoNE, ii, jj, kk) = TMP1_XONE + TMP2_XONE + TMP3_XONE + TMP4_XONE
02476         + TMP5_XONE + TMP6_XONE;
02477
02478     //fprintf(data, "%19.12E\n", VAT3(XoNE, ii, jj, kk));
02479
02480     /* *****
02481      * *** > ONW;
02482      * *****
02483
02484     // VAT3(XoNW, ii, jj, kk) =
02485     TMP1_XONW =
02486         - VAT3( dPW, ii, jj, kk) * (- VAT3( oNW, im1, j, km1) * VAT3( dPS, iim1, jjp1, kk)
02487             - VAT3( uNW, im1, j, km1) * VAT3( oPS, iim1, jjp1, kk)
02488             - VAT3( oN, im1, j, km1) * VAT3( dPSE, iim1, jjp1, kk)
02489             - VAT3( uN, im1, j, km1) * VAT3( oPSE, iim1, jjp1, kk))
02490
02491         - VAT3( oPW, ii, jj, kk) * (- VAT3( uSE, im2, jp1, km1) * VAT3( dPS, iim1, jjp1, kk)
02492             - VAT3( oNW, im1, j, k) * VAT3( oPS, iim1, jjp1, kk)
02493             - VAT3( uNW, im1, j, k) * VAT3( uPS, iim1, jjp1, kk)
02494             - VAT3( uS, im1, jp1, km1) * VAT3( dPSE, iim1, jjp1, kk)
02495             - VAT3( oN, im1, j, k) * VAT3( oPSE, iim1, jjp1, kk)
02496             - VAT3( uN, im1, j, k) * VAT3( uPSE, iim1, jjp1, kk));
02497
02498     TMP2_XONW =
02499         - VAT3( oPW, ii, jj, kk) * (- VAT3( uSE, im2, jp1, k) * VAT3( oPS, iim1, jjp1, kk)
02500             - VAT3( oNW, im1, j, kp1) * VAT3( uPS, iim1, jjp1, kk)
02501             - VAT3( uS, im1, jp1, k) * VAT3( oPSE, iim1, jjp1, kk)
02502             - VAT3( oN, im1, j, kp1) * VAT3( uPSE, iim1, jjp1, kk))
02503
02504         - VAT3( dPNW, ii, jj, kk) * (- VAT3( oE, im2, jp1, km1) * VAT3( dPS, iim1, jjp1, kk)
02505             - VAT3( uW, im1, jp1, km1) * VAT3( oPS, iim1, jjp1, kk)
02506             - VAT3( oNW, im1, jp1, km1) * VAT3( dPC, iim1, jjp1, kk)
02507             - VAT3( uNW, im1, jp1, km1) * VAT3( oPC, iim1, jjp1, kk)
02508             + VAT3( oC, im1, jp1, km1) * VAT3( dPSE, iim1, jjp1, kk)
02509             - VAT3( uC, im1, jp1, km1) * VAT3( oPSE, iim1, jjp1, kk)
02510             - VAT3( oN, im1, jp1, km1) * VAT3( dPE, iim1, jjp1, kk)
02511             - VAT3( uN, im1, jp1, km1) * VAT3( oPE, iim1, jjp1, kk));
02512
02513     TMP3_XONW =
02514         - VAT3( oPNW, ii, jj, kk) * (- VAT3( uE, im2, jp1, km1) * VAT3( dPS, iim1, jjp1, kk)
02515             - VAT3( oE, im2, jp1, k) * VAT3( oPS, iim1, jjp1, kk)
02516             - VAT3( uW, im1, jp1, k) * VAT3( uPS, iim1, jjp1, kk)
02517             - VAT3( uSE, im2, jp2, km1) * VAT3( dPC, iim1, jjp1, kk)
02518             - VAT3( oNW, im1, jp1, k) * VAT3( oPC, iim1, jjp1, kk)
02519             - VAT3( uNW, im1, jp1, k) * VAT3( uPC, iim1, jjp1, kk)
02520             - VAT3( uC, im1, jp1, km1) * VAT3( dPSE, iim1, jjp1, kk)
02521             + VAT3( oC, im1, jp1, k) * VAT3( oPSE, iim1, jjp1, kk)
02522             - VAT3( uC, im1, jp1, k) * VAT3( uPSE, iim1, jjp1, kk)
02523             - VAT3( uS, im1, jp2, km1) * VAT3( dPE, iim1, jjp1, kk)
02524             - VAT3( oN, im1, jp1, k) * VAT3( oPE, iim1, jjp1, kk)
02525             - VAT3( uN, im1, jp1, k) * VAT3( uPE, iim1, jjp1, kk));
02526
02527     TMP4_XONW =
02528         - VAT3( uPNW, ii, jj, kk) * (- VAT3( uE, im2, jp1, k) * VAT3( oPS, iim1, jjp1, kk)
02529             - VAT3( oE, im2, jp1, kp1) * VAT3( uPS, iim1, jjp1, kk)
02530             - VAT3( uSE, im2, jp2, k) * VAT3( oPC, iim1, jjp1, kk)
02531             - VAT3( oNW, im1, jp1, kp1) * VAT3( uPC, iim1, jjp1, kk)
02532             - VAT3( uC, im1, jp1, k) * VAT3( oPSE, iim1, jjp1, kk)
02533             + VAT3( oC, im1, jp1, kp1) * VAT3( uPSE, iim1, jjp1, kk)
02534             - VAT3( uS, im1, jp2, k) * VAT3( oPE, iim1, jjp1, kk)
02535             - VAT3( oN, im1, jp1, kp1) * VAT3( uPE, iim1, jjp1, kk))
02536
02537         - VAT3( dPC, ii, jj, kk) * (- VAT3( oNW, i, j, km1) * VAT3( dPSE, iim1, jjp1, kk)
02538             - VAT3( uNW, i, j, km1) * VAT3( oPSE, iim1, jjp1, kk));
02539
02540     TMP5_XONW =
02541         - VAT3( oPC, ii, jj, kk) * (- VAT3( uSE, im1, jp1, km1) * VAT3( dPSE, iim1, jjp1, kk)
02542             - VAT3( oNW, i, j, k) * VAT3( oPSE, iim1, jjp1, kk)
02543             - VAT3( uNW, i, j, k) * VAT3( uPSE, iim1, jjp1, kk))
02544

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02545     - VAT3( uPC, ii,jj,kk) * (- VAT3( uSE, im1,jp1,k) * VAT3(oPSE, iim1,jjp1,kk)
02546         - VAT3( oNW, i,j,kp1) * VAT3(uPSE, iim1,jjp1,kk))
02547
02548     - VAT3( dPN, ii,jj,kk) * (- VAT3( oE, im1,jp1,km1) * VAT3(dPSE, iim1,jjp1,kk)
02549         - VAT3( uW, i,jp1,km1) * VAT3(oPSE, iim1,jjp1,kk)
02550         - VAT3( oNW, i,jp1,km1) * VAT3( dPE, iim1,jjp1,kk)
02551         - VAT3( uNW, i,jp1,km1) * VAT3( oPE, iim1,jjp1,kk));
02552
02553 TMP6_XONW =
02554     - VAT3( oPN, ii,jj,kk) * (- VAT3( uE, im1,jp1,km1) * VAT3(dPSE, iim1,jjp1,kk)
02555         - VAT3( oE, im1,jp1,k) * VAT3(oPSE, iim1,jjp1,kk)
02556         - VAT3( uW, i,jp1,k) * VAT3(uPSE, iim1,jjp1,kk)
02557         - VAT3( uSE, im1,jp2,km1) * VAT3( dPE, iim1,jjp1,kk)
02558         - VAT3( oNW, i,jp1,k) * VAT3( oPE, iim1,jjp1,kk)
02559         - VAT3( uNW, i,jp1,k) * VAT3( uPE, iim1,jjp1,kk))
02560
02561     - VAT3( uPN, ii,jj,kk) * (- VAT3( uE, im1,jp1,k) * VAT3(oPSE, iim1,jjp1,kk)
02562         - VAT3( oE, im1,jp1,kp1) * VAT3(uPSE, iim1,jjp1,kk)
02563         - VAT3( uSE, im1,jp2,k) * VAT3( oPE, iim1,jjp1,kk)
02564         - VAT3( oNW, i,jp1,kp1) * VAT3( uPE, iim1,jjp1,kk));
02565
02566 VAT3(XoNW, ii,jj,kk) = TMP1_XONW + TMP2_XONW + TMP3_XONW + TMP4_XONW
02567     + TMP5_XONW + TMP6_XONW;
02568
02569 //fprintf(data, "%19.12E\n", VAT3(XoNW, ii, jj, kk));
02570
02571 /* *****
02572  * *** > UE;
02573  * *****
02574  // VAT3( XuE, ii,jj,kk) =
02575 TMP1_XUE =
02576     - VAT3( oPS, ii,jj,kk) * (- VAT3( uE, i,jm1,k) * VAT3(dPSW, iip1,jj,kkp1)
02577         - VAT3( uNE, i,jm1,k) * VAT3( dPW, iip1,jj,kkp1))
02578
02579     - VAT3( uPS, ii,jj,kk) * (- VAT3( oE, i,jm1,kp1) * VAT3(dPSW, iip1,jj,kkp1)
02580         - VAT3( uE, i,jm1,kp1) * VAT3(oPSW, iip1,jj,kkp1)
02581         - VAT3( oNE, i,jm1,kp1) * VAT3( dPW, iip1,jj,kkp1)
02582         - VAT3( uNE, i,jm1,kp1) * VAT3( oPW, iip1,jj,kkp1))
02583
02584     - VAT3( oPC, ii,jj,kk) * (- VAT3( uSE, i,j,k) * VAT3(dPSW, iip1,jj,kkp1)
02585         - VAT3( uE, i,j,k) * VAT3( dPW, iip1,jj,kkp1)
02586         - VAT3( uNE, i,j,k) * VAT3(dPNW, iip1,jj,kkp1));
02587
02588 TMP2_XUE =
02589     - VAT3( uPC, ii,jj,kk) * (- VAT3( oNW, ip1,jm1,kp1) * VAT3(dPSW, iip1,jj,kkp1)
02590         - VAT3( uSE, i,j,kp1) * VAT3(oPSW, iip1,jj,kkp1)
02591         - VAT3( oE, i,j,kp1) * VAT3( dPW, iip1,jj,kkp1)
02592         - VAT3( uE, i,j,kp1) * VAT3( oPW, iip1,jj,kkp1)
02593         - VAT3( oNE, i,j,kp1) * VAT3(dPNW, iip1,jj,kkp1)
02594         - VAT3( uNE, i,j,kp1) * VAT3(oPNW, iip1,jj,kkp1))
02595
02596     - VAT3( oPN, ii,jj,kk) * (- VAT3( uSE, i,jp1,k) * VAT3( dPW, iip1,jj,kkp1)
02597         - VAT3( uE, i,jp1,k) * VAT3(dPNW, iip1,jj,kkp1))
02598
02599     - VAT3( uPN, ii,jj,kk) * (- VAT3( oNW, ip1,j,kp1) * VAT3( dPW, iip1,jj,kkp1)
02600         - VAT3( uSE, i,jp1,kp1) * VAT3( oPW, iip1,jj,kkp1)
02601         - VAT3( oE, i,jp1,kp1) * VAT3(dPNW, iip1,jj,kkp1)
02602         - VAT3( uE, i,jp1,kp1) * VAT3(oPNW, iip1,jj,kkp1));
02603
02604 TMP3_XUE =
02605     - VAT3(oPSE, ii,jj,kk) * (- VAT3( uC, ip1,jm1,k) * VAT3(dPSW, iip1,jj,kkp1)
02606         - VAT3( uN, ip1,jm1,k) * VAT3( dPW, iip1,jj,kkp1)
02607         - VAT3( uE, ip1,jm1,k) * VAT3( dPS, iip1,jj,kkp1)
02608         - VAT3( uNE, ip1,jm1,k) * VAT3( dPC, iip1,jj,kkp1))
02609
02610     - VAT3(uPSE, ii,jj,kk) * ( VAT3( oC, ip1,jm1,kp1) * VAT3(dPSW, iip1,jj,kkp1)
02611         - VAT3( uC, ip1,jm1,kp1) * VAT3(oPSW, iip1,jj,kkp1)
02612         - VAT3( oN, ip1,jm1,kp1) * VAT3( dPW, iip1,jj,kkp1)
02613         - VAT3( uN, ip1,jm1,kp1) * VAT3( oPW, iip1,jj,kkp1)
02614         - VAT3( oE, ip1,jm1,kp1) * VAT3( dPS, iip1,jj,kkp1)
02615         - VAT3( uE, ip1,jm1,kp1) * VAT3( oPS, iip1,jj,kkp1)
02616         - VAT3( oNE, ip1,jm1,kp1) * VAT3( dPC, iip1,jj,kkp1)
02617         - VAT3( uNE, ip1,jm1,kp1) * VAT3( oPC, iip1,jj,kkp1));
02618
02619 TMP4_XUE =
02620     - VAT3( oPE, ii,jj,kk) * (- VAT3( uS, ip1,j,k) * VAT3(dPSW, iip1,jj,kkp1)
02621         - VAT3( uC, ip1,j,k) * VAT3( dPW, iip1,jj,kkp1)
02622         - VAT3( uN, ip1,j,k) * VAT3(dPNW, iip1,jj,kkp1)
02623         - VAT3( uSE, ip1,j,k) * VAT3( dPS, iip1,jj,kkp1)
02624         - VAT3( uE, ip1,j,k) * VAT3( dPC, iip1,jj,kkp1)
02625         - VAT3( uNE, ip1,j,k) * VAT3( dPN, iip1,jj,kkp1));

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02626
02627     TMP5_XUE =
02628         - VAT3( uPE, ii,jj,kk) * ( - VAT3( oN, ip1,jml,kp1) * VAT3(dPSW, iip1,jj,kkp1)
02629             - VAT3( uS, ip1,j,kp1) * VAT3(oPSW, iip1,jj,kkp1)
02630             + VAT3( oC, ip1,j,kp1) * VAT3( dPW, iip1,jj,kkp1)
02631             - VAT3( uC, ip1,j,kp1) * VAT3( oPW, iip1,jj,kkp1)
02632             - VAT3( oN, ip1,j,kp1) * VAT3(dPNW, iip1,jj,kkp1)
02633             - VAT3( uN, ip1,j,kp1) * VAT3(oPNW, iip1,jj,kkp1)
02634             - VAT3( oNW, ip2,jml,kp1) * VAT3( dPS, iip1,jj,kkp1)
02635             - VAT3( uSE, ip1,j,kp1) * VAT3( oPS, iip1,jj,kkp1)
02636             - VAT3( oE, ip1,j,kp1) * VAT3( dPC, iip1,jj,kkp1)
02637             - VAT3( uE, ip1,j,kp1) * VAT3( oPC, iip1,jj,kkp1)
02638             - VAT3( oNE, ip1,j,kp1) * VAT3( dPN, iip1,jj,kkp1)
02639             - VAT3( uNE, ip1,j,kp1) * VAT3( oPN, iip1,jj,kkp1));
02640
02641     TMP6_XUE =
02642         - VAT3(oPNE, ii,jj,kk) * ( - VAT3( uS, ip1,jp1,k) * VAT3( dPW, iip1,jj,kkp1)
02643             - VAT3( uC, ip1,jp1,k) * VAT3(dPNW, iip1,jj,kkp1)
02644             - VAT3( uSE, ip1,jp1,k) * VAT3( dPC, iip1,jj,kkp1)
02645             - VAT3( uE, ip1,jp1,k) * VAT3( dPN, iip1,jj,kkp1))
02646
02647         - VAT3(uPNE, ii,jj,kk) * ( - VAT3( oN, ip1,j,kp1) * VAT3( dPW, iip1,jj,kkp1)
02648             - VAT3( uS, ip1,jp1,kp1) * VAT3( oPW, iip1,jj,kkp1)
02649             + VAT3( oC, ip1,jp1,kp1) * VAT3(dPNW, iip1,jj,kkp1)
02650             - VAT3( uC, ip1,jp1,kp1) * VAT3(oPNW, iip1,jj,kkp1)
02651             - VAT3( oNW, ip2,j,kp1) * VAT3( dPC, iip1,jj,kkp1)
02652             - VAT3( uSE, ip1,jp1,kp1) * VAT3( oPC, iip1,jj,kkp1)
02653             - VAT3( oE, ip1,jp1,kp1) * VAT3( dPN, iip1,jj,kkp1)
02654             - VAT3( uE, ip1,jp1,kp1) * VAT3( oPN, iip1,jj,kkp1));
02655
02656     VAT3( XuE, ii,jj,kk) = TMP1_XUE + TMP2_XUE + TMP3_XUE + TMP4_XUE
02657         + TMP5_XUE + TMP6_XUE;
02658
02659     //fprintf(data, "%19.12E\n", VAT3(XuE, ii, jj, kk));
02660
02661     /* *****
02662      * *** > UW;
02663      * *****
02664      // VAT3( XuW, ii,jj,kk) =
02665     TMP1_XUW =
02666         - VAT3(oPSW, ii,jj,kk) * ( - VAT3( uW, im1,jml,k) * VAT3( dPS, iim1,jj,kkp1)
02667             - VAT3( uNW, im1,jml,k) * VAT3( dPC, iim1,jj,kkp1)
02668             - VAT3( uC, im1,jml,k) * VAT3(dPSE, iim1,jj,kkp1)
02669             - VAT3( uN, im1,jml,k) * VAT3( dPE, iim1,jj,kkp1))
02670
02671         - VAT3(uPSW, ii,jj,kk) * ( - VAT3( oE, im2,jml,kp1) * VAT3( dPS, iim1,jj,kkp1)
02672             - VAT3( uW, im1,jml,kp1) * VAT3( oPS, iim1,jj,kkp1)
02673             - VAT3( oNW, im1,jml,kp1) * VAT3( dPC, iim1,jj,kkp1)
02674             - VAT3( uNW, im1,jml,kp1) * VAT3( oPC, iim1,jj,kkp1)
02675             + VAT3( oC, im1,jml,kp1) * VAT3(dPSE, iim1,jj,kkp1)
02676             - VAT3( uC, im1,jml,kp1) * VAT3(oPSE, iim1,jj,kkp1)
02677             - VAT3( oN, im1,jml,kp1) * VAT3( dPE, iim1,jj,kkp1)
02678             - VAT3( uN, im1,jml,kp1) * VAT3( oPE, iim1,jj,kkp1));
02679
02680     TMP2_XUW =
02681         - VAT3( oPW, ii,jj,kk) * ( - VAT3( uSW, im1,j,k) * VAT3( dPS, iim1,jj,kkp1)
02682             - VAT3( uW, im1,j,k) * VAT3( dPC, iim1,jj,kkp1)
02683             - VAT3( uNW, im1,j,k) * VAT3( dPN, iim1,jj,kkp1)
02684             - VAT3( uS, im1,j,k) * VAT3(dPSE, iim1,jj,kkp1)
02685             - VAT3( uC, im1,j,k) * VAT3( dPE, iim1,jj,kkp1)
02686             - VAT3( uN, im1,j,k) * VAT3(dPNE, iim1,jj,kkp1));
02687
02688     TMP3_XUW =
02689         - VAT3( uPW, ii,jj,kk) * ( - VAT3( oNE, im2,jml,kp1) * VAT3( dPS, iim1,jj,kkp1)
02690             - VAT3( uSW, im1,j,kp1) * VAT3( oPS, iim1,jj,kkp1)
02691             - VAT3( oE, im2,j,kp1) * VAT3( dPC, iim1,jj,kkp1)
02692             - VAT3( uW, im1,j,kp1) * VAT3( oPC, iim1,jj,kkp1)
02693             - VAT3( oNW, im1,j,kp1) * VAT3( dPN, iim1,jj,kkp1)
02694             - VAT3( uNW, im1,j,kp1) * VAT3( oPN, iim1,jj,kkp1)
02695             - VAT3( oN, im1,jml,kp1) * VAT3(dPSE, iim1,jj,kkp1)
02696             - VAT3( uS, im1,j,kp1) * VAT3(oPSE, iim1,jj,kkp1)
02697             + VAT3( oC, im1,j,kp1) * VAT3( dPE, iim1,jj,kkp1)
02698             - VAT3( uC, im1,j,kp1) * VAT3( oPE, iim1,jj,kkp1)
02699             - VAT3( oN, im1,j,kp1) * VAT3(dPNE, iim1,jj,kkp1)
02700             - VAT3( uN, im1,j,kp1) * VAT3(oPNE, iim1,jj,kkp1));
02701
02702     TMP4_XUW =
02703         - VAT3(oPNW, ii,jj,kk) * ( - VAT3( uSW, im1,jp1,k) * VAT3( dPC, iim1,jj,kkp1)
02704             - VAT3( uW, im1,jp1,k) * VAT3( dPN, iim1,jj,kkp1)
02705             - VAT3( uS, im1,jp1,k) * VAT3( dPE, iim1,jj,kkp1)
02706             - VAT3( uC, im1,jp1,k) * VAT3(dPNE, iim1,jj,kkp1))

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02707
02708 - VAT3( uPNW, ii, jj, kk) * (- VAT3( oNE, im2, j, kp1) * VAT3( dPC, iim1, jj, kkp1)
02709 - VAT3( uSW, im1, jpl, kp1) * VAT3( oPC, iim1, jj, kkp1)
02710 - VAT3( oE, im2, jpl, kp1) * VAT3( dPN, iim1, jj, kkp1)
02711 - VAT3( uW, im1, jpl, kp1) * VAT3( oPN, iim1, jj, kkp1)
02712 - VAT3( oN, im1, j, kp1) * VAT3( dPE, iim1, jj, kkp1)
02713 - VAT3( uS, im1, jpl, kp1) * VAT3( oPE, iim1, jj, kkp1)
02714 + VAT3( oC, im1, jpl, kp1) * VAT3( dPNE, iim1, jj, kkp1)
02715 - VAT3( uC, im1, jpl, kp1) * VAT3( oPNE, iim1, jj, kkp1));
02716
02717 TMP5_XUW =
02718 - VAT3( oPS, ii, jj, kk) * (- VAT3( uW, i, jml, k) * VAT3( dPSE, iim1, jj, kkp1)
02719 - VAT3( uNW, i, jml, k) * VAT3( dPE, iim1, jj, kkp1))
02720
02721 - VAT3( uPS, ii, jj, kk) * (- VAT3( oE, im1, jml, kp1) * VAT3( dPSE, iim1, jj, kkp1)
02722 - VAT3( uW, i, jml, kp1) * VAT3( oPSE, iim1, jj, kkp1)
02723 - VAT3( oNW, i, jml, kp1) * VAT3( dPE, iim1, jj, kkp1)
02724 - VAT3( uNW, i, jml, kp1) * VAT3( oPE, iim1, jj, kkp1))
02725
02726 - VAT3( oPC, ii, jj, kk) * (- VAT3( uSW, i, j, k) * VAT3( dPSE, iim1, jj, kkp1)
02727 - VAT3( uW, i, j, k) * VAT3( dPE, iim1, jj, kkp1)
02728 - VAT3( uNW, i, j, k) * VAT3( dPNE, iim1, jj, kkp1));
02729
02730 TMP6_XUW =
02731 - VAT3( uPC, ii, jj, kk) * (- VAT3( oNE, im1, jml, kp1) * VAT3( dPSE, iim1, jj, kkp1)
02732 - VAT3( uSW, i, j, kp1) * VAT3( oPSE, iim1, jj, kkp1)
02733 - VAT3( oE, im1, j, kp1) * VAT3( dPE, iim1, jj, kkp1)
02734 - VAT3( uW, i, j, kp1) * VAT3( oPE, iim1, jj, kkp1)
02735 - VAT3( oNW, i, j, kp1) * VAT3( dPNE, iim1, jj, kkp1)
02736 - VAT3( uNW, i, j, kp1) * VAT3( oPNE, iim1, jj, kkp1))
02737
02738 - VAT3( oPN, ii, jj, kk) * (- VAT3( uSW, i, jpl, k) * VAT3( dPE, iim1, jj, kkp1)
02739 - VAT3( uW, i, jpl, k) * VAT3( dPNE, iim1, jj, kkp1))
02740
02741 - VAT3( uPN, ii, jj, kk) * (- VAT3( oNE, im1, j, kp1) * VAT3( dPE, iim1, jj, kkp1)
02742 - VAT3( uSW, i, jpl, kp1) * VAT3( oPE, iim1, jj, kkp1)
02743 - VAT3( oE, im1, jpl, kp1) * VAT3( dPNE, iim1, jj, kkp1)
02744 - VAT3( uW, i, jpl, kp1) * VAT3( oPNE, iim1, jj, kkp1));
02745
02746 VAT3( XuW, ii, jj, kk) = TMP1_XUW + TMP2_XUW + TMP3_XUW + TMP4_XUW
02747 + TMP5_XUW + TMP6_XUW;
02748
02749 //fprintf(data, "%19.12E\n", VAT3(XuW, ii, jj, kk));
02750
02751 /* *****
02752 * *** > UN;
02753 * *****
02754 // VAT3( XuN, ii, jj, kk) =
02755 TMP1_XUN =
02756 - VAT3( oPW, ii, jj, kk) * (- VAT3( uN, im1, j, k) * VAT3( dPSW, ii, jjpl, kkp1)
02757 - VAT3( uNE, im1, j, k) * VAT3( dPS, ii, jjpl, kkp1))
02758
02759 - VAT3( uPW, ii, jj, kk) * (- VAT3( oN, im1, j, kp1) * VAT3( dPSW, ii, jjpl, kkp1)
02760 - VAT3( uN, im1, j, kp1) * VAT3( oPSW, ii, jjpl, kkp1)
02761 - VAT3( oNE, im1, j, kp1) * VAT3( dPS, ii, jjpl, kkp1)
02762 - VAT3( uNE, im1, j, kp1) * VAT3( oPS, ii, jjpl, kkp1))
02763
02764 - VAT3( oPNW, ii, jj, kk) * (- VAT3( uC, im1, jpl, k) * VAT3( dPSW, ii, jjpl, kkp1)
02765 - VAT3( uN, im1, jpl, k) * VAT3( dPW, ii, jjpl, kkp1)
02766 - VAT3( uE, im1, jpl, k) * VAT3( dPS, ii, jjpl, kkp1)
02767 - VAT3( uNE, im1, jpl, k) * VAT3( dPC, ii, jjpl, kkp1));
02768
02769 TMP2_XUN =
02770 - VAT3( uPNW, ii, jj, kk) * ( VAT3( oC, im1, jpl, kp1) * VAT3( dPSW, ii, jjpl, kkp1)
02771 - VAT3( uC, im1, jpl, kp1) * VAT3( oPSW, ii, jjpl, kkp1)
02772 - VAT3( oN, im1, jpl, kp1) * VAT3( dPW, ii, jjpl, kkp1)
02773 - VAT3( uN, im1, jpl, kp1) * VAT3( oPW, ii, jjpl, kkp1)
02774 - VAT3( oE, im1, jpl, kp1) * VAT3( dPS, ii, jjpl, kkp1)
02775 - VAT3( uE, im1, jpl, kp1) * VAT3( oPS, ii, jjpl, kkp1)
02776 - VAT3( oNE, im1, jpl, kp1) * VAT3( dPC, ii, jjpl, kkp1)
02777 - VAT3( uNE, im1, jpl, kp1) * VAT3( oPC, ii, jjpl, kkp1))
02778
02779 - VAT3( oPC, ii, jj, kk) * (- VAT3( uNW, i, j, k) * VAT3( dPSW, ii, jjpl, kkp1)
02780 - VAT3( uN, i, j, k) * VAT3( dPS, ii, jjpl, kkp1)
02781 - VAT3( uNE, i, j, k) * VAT3( dPSE, ii, jjpl, kkp1));
02782
02783 TMP3_XUN =
02784 - VAT3( uPC, ii, jj, kk) * (- VAT3( oNW, i, j, kp1) * VAT3( dPSW, ii, jjpl, kkp1)
02785 - VAT3( uNW, i, j, kp1) * VAT3( oPSW, ii, jjpl, kkp1)
02786 - VAT3( oN, i, j, kp1) * VAT3( dPS, ii, jjpl, kkp1)
02787 - VAT3( uN, i, j, kp1) * VAT3( oPS, ii, jjpl, kkp1)

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02788             - VAT3( oNE, i, j, kp1) * VAT3( dPSE, ii, jjp1, kkp1)
02789             - VAT3( uNE, i, j, kp1) * VAT3( oPSE, ii, jjp1, kkp1))
02790
02791         - VAT3( oPN, ii, jj, kk) * (- VAT3( uW, i, jp1, k) * VAT3( dPSW, ii, jjp1, kkp1)
02792             - VAT3( uNW, i, jp1, k) * VAT3( dPW, ii, jjp1, kkp1)
02793             - VAT3( uC, i, jp1, k) * VAT3( dPS, ii, jjp1, kkp1)
02794             - VAT3( uN, i, jp1, k) * VAT3( dPC, ii, jjp1, kkp1)
02795             - VAT3( uE, i, jp1, k) * VAT3( dPSE, ii, jjp1, kkp1)
02796             - VAT3( uNE, i, jp1, k) * VAT3( dPE, ii, jjp1, kkp1));
02797
02798     TMP4_XUN =
02799         - VAT3( uPN, ii, jj, kk) * (- VAT3( oE, im1, jp1, kp1) * VAT3( dPSW, ii, jjp1, kkp1)
02800             - VAT3( uW, i, jp1, kp1) * VAT3( oPSW, ii, jjp1, kkp1)
02801             - VAT3( oNW, i, jp1, kp1) * VAT3( dPW, ii, jjp1, kkp1)
02802             - VAT3( uNW, i, jp1, kp1) * VAT3( oPW, ii, jjp1, kkp1)
02803             + VAT3( oC, i, jp1, kp1) * VAT3( dPS, ii, jjp1, kkp1)
02804             - VAT3( uC, i, jp1, kp1) * VAT3( oPS, ii, jjp1, kkp1)
02805             - VAT3( oN, i, jp1, kp1) * VAT3( dPC, ii, jjp1, kkp1)
02806             - VAT3( uN, i, jp1, kp1) * VAT3( oPC, ii, jjp1, kkp1)
02807             - VAT3( oE, i, jp1, kp1) * VAT3( dPSE, ii, jjp1, kkp1)
02808             - VAT3( uE, i, jp1, kp1) * VAT3( oPSE, ii, jjp1, kkp1)
02809             - VAT3( oNE, i, jp1, kp1) * VAT3( dPE, ii, jjp1, kkp1)
02810             - VAT3( uNE, i, jp1, kp1) * VAT3( oPE, ii, jjp1, kkp1));
02811
02812     TMP5_XUN =
02813         - VAT3( oPE, ii, jj, kk) * (- VAT3( uNW, ip1, j, k) * VAT3( dPS, ii, jjp1, kkp1)
02814             - VAT3( uN, ip1, j, k) * VAT3( dPSE, ii, jjp1, kkp1))
02815
02816         - VAT3( uPE, ii, jj, kk) * (- VAT3( oNW, ip1, j, kp1) * VAT3( dPS, ii, jjp1, kkp1)
02817             - VAT3( uNW, ip1, j, kp1) * VAT3( oPS, ii, jjp1, kkp1)
02818             - VAT3( oN, ip1, j, kp1) * VAT3( dPSE, ii, jjp1, kkp1)
02819             - VAT3( uN, ip1, j, kp1) * VAT3( oPSE, ii, jjp1, kkp1))
02820
02821         - VAT3( oPNE, ii, jj, kk) * (- VAT3( uW, ip1, jp1, k) * VAT3( dPS, ii, jjp1, kkp1)
02822             - VAT3( uNW, ip1, jp1, k) * VAT3( dPC, ii, jjp1, kkp1)
02823             - VAT3( uC, ip1, jp1, k) * VAT3( dPSE, ii, jjp1, kkp1)
02824             - VAT3( uN, ip1, jp1, k) * VAT3( dPE, ii, jjp1, kkp1));
02825
02826     TMP6_XUN =
02827         - VAT3( uPNE, ii, jj, kk) * (- VAT3( oE, i, jp1, kp1) * VAT3( dPS, ii, jjp1, kkp1)
02828             - VAT3( uW, ip1, jp1, kp1) * VAT3( oPS, ii, jjp1, kkp1)
02829             - VAT3( oNW, ip1, jp1, kp1) * VAT3( dPC, ii, jjp1, kkp1)
02830             - VAT3( uNW, ip1, jp1, kp1) * VAT3( oPC, ii, jjp1, kkp1)
02831             + VAT3( oC, ip1, jp1, kp1) * VAT3( dPSE, ii, jjp1, kkp1)
02832             - VAT3( uC, ip1, jp1, kp1) * VAT3( oPSE, ii, jjp1, kkp1)
02833             - VAT3( oN, ip1, jp1, kp1) * VAT3( dPE, ii, jjp1, kkp1)
02834             - VAT3( uN, ip1, jp1, kp1) * VAT3( oPE, ii, jjp1, kkp1));
02835
02836     VAT3( XuN, ii, jj, kk) = TMP1_XUN + TMP2_XUN + TMP3_XUN + TMP4_XUN
02837         + TMP5_XUN + TMP6_XUN;
02838
02839     //fprintf(data, "%19.12E\n", VAT3(XuN, ii, jj, kk));
02840
02841     /* *****
02842      * *** > US;
02843      * *****/
02844
02845     // VAT3( XuS, ii, jj, kk) =
02846     TMP1_XUS =
02847         - VAT3( oPSW, ii, jj, kk) * (- VAT3( uS, im1, jml, k) * VAT3( dPW, ii, jjml, kkp1)
02848             - VAT3( uC, im1, jml, k) * VAT3( dPNW, ii, jjml, kkp1)
02849             - VAT3( uSE, im1, jml, k) * VAT3( dPC, ii, jjml, kkp1)
02850             - VAT3( uE, im1, jml, k) * VAT3( dPN, ii, jjml, kkp1))
02851
02852         - VAT3( uPSW, ii, jj, kk) * (- VAT3( oN, im1, jm2, kp1) * VAT3( dPW, ii, jjml, kkp1)
02853             - VAT3( uS, im1, jml, kp1) * VAT3( oPW, ii, jjml, kkp1)
02854             + VAT3( oC, im1, jml, kp1) * VAT3( dPNW, ii, jjml, kkp1)
02855             - VAT3( uC, im1, jml, kp1) * VAT3( oPNW, ii, jjml, kkp1)
02856             - VAT3( oNW, i, jm2, kp1) * VAT3( dPC, ii, jjml, kkp1)
02857             - VAT3( uSE, im1, jml, kp1) * VAT3( oPC, ii, jjml, kkp1)
02858             - VAT3( oE, im1, jml, kp1) * VAT3( dPN, ii, jjml, kkp1)
02859             - VAT3( uE, im1, jml, kp1) * VAT3( oPN, ii, jjml, kkp1));
02860
02861     TMP2_XUS =
02862         - VAT3( oPW, ii, jj, kk) * (- VAT3( uS, im1, j, k) * VAT3( dPNW, ii, jjml, kkp1)
02863             - VAT3( uSE, im1, j, k) * VAT3( dPN, ii, jjml, kkp1))
02864
02865         - VAT3( uPW, ii, jj, kk) * (- VAT3( oN, im1, jml, kp1) * VAT3( dPNW, ii, jjml, kkp1)
02866             - VAT3( uS, im1, j, kp1) * VAT3( oPNW, ii, jjml, kkp1)
02867             - VAT3( oNW, i, jml, kp1) * VAT3( dPN, ii, jjml, kkp1)
02868             - VAT3( uSE, im1, j, kp1) * VAT3( oPN, ii, jjml, kkp1))

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02869
02870 - VAT3( oPS, ii,jj,kk) * (- VAT3( uSW, i,jm1,k) * VAT3( dPW, ii,jjm1,kkp1)
02871 - VAT3( uW, i,jm1,k) * VAT3( dPNW, ii,jjm1,kkp1)
02872 - VAT3( uS, i,jm1,k) * VAT3( dPC, ii,jjm1,kkp1)
02873 - VAT3( uC, i,jm1,k) * VAT3( dPN, ii,jjm1,kkp1)
02874 - VAT3( uSE, i,jm1,k) * VAT3( dPE, ii,jjm1,kkp1)
02875 - VAT3( uE, i,jm1,k) * VAT3( dPNE, ii,jjm1,kkp1));
02876
02877 TMP3_XUS =
02878 - VAT3( uPS, ii,jj,kk) * (- VAT3( oNE, im1,jm2,kp1) * VAT3( dPW, ii,jjm1,kkp1)
02879 - VAT3( uSW, i,jm1,kp1) * VAT3( oPW, ii,jjm1,kkp1)
02880 - VAT3( oE, im1,jm1,kp1) * VAT3( dPNW, ii,jjm1,kkp1)
02881 - VAT3( uW, i,jm1,kp1) * VAT3( oPNW, ii,jjm1,kkp1)
02882 - VAT3( oN, i,jm2,kp1) * VAT3( dPC, ii,jjm1,kkp1)
02883 - VAT3( uS, i,jm1,kp1) * VAT3( oPC, ii,jjm1,kkp1)
02884 + VAT3( oC, i,jm1,kp1) * VAT3( dPN, ii,jjm1,kkp1)
02885 - VAT3( uC, i,jm1,kp1) * VAT3( oPN, ii,jjm1,kkp1)
02886 - VAT3( oNW, ip1,jm2,kp1) * VAT3( dPE, ii,jjm1,kkp1)
02887 - VAT3( uSE, i,jm1,kp1) * VAT3( oPE, ii,jjm1,kkp1)
02888 - VAT3( oE, i,jm1,kp1) * VAT3( dPNE, ii,jjm1,kkp1)
02889 - VAT3( uE, i,jm1,kp1) * VAT3( oPNE, ii,jjm1,kkp1));
02890
02891 TMP4_XUS =
02892 - VAT3( oPC, ii,jj,kk) * (- VAT3( uSW, i,j,k) * VAT3( dPNW, ii,jjm1,kkp1)
02893 - VAT3( uS, i,j,k) * VAT3( dPN, ii,jjm1,kkp1)
02894 - VAT3( uSE, i,j,k) * VAT3( dPNE, ii,jjm1,kkp1))
02895
02896 - VAT3( uPC, ii,jj,kk) * (- VAT3( oNE, im1,jm1,kp1) * VAT3( dPNW, ii,jjm1,kkp1)
02897 - VAT3( uSW, i,j,kp1) * VAT3( oPNW, ii,jjm1,kkp1)
02898 - VAT3( oN, i,jm1,kp1) * VAT3( dPN, ii,jjm1,kkp1)
02899 - VAT3( uS, i,j,kp1) * VAT3( oPN, ii,jjm1,kkp1)
02900 - VAT3( oNW, ip1,jm1,kp1) * VAT3( dPNE, ii,jjm1,kkp1)
02901 - VAT3( uSE, i,j,kp1) * VAT3( oPNE, ii,jjm1,kkp1));
02902
02903 TMP5_XUS =
02904 - VAT3( oPSE, ii,jj,kk) * (- VAT3( uSW, ip1,jm1,k) * VAT3( dPC, ii,jjm1,kkp1)
02905 - VAT3( uW, ip1,jm1,k) * VAT3( dPN, ii,jjm1,kkp1)
02906 - VAT3( uS, ip1,jm1,k) * VAT3( dPE, ii,jjm1,kkp1)
02907 - VAT3( uC, ip1,jm1,k) * VAT3( dPNE, ii,jjm1,kkp1))
02908
02909 - VAT3( uPSE, ii,jj,kk) * (- VAT3( oNE, i,jm2,kp1) * VAT3( dPC, ii,jjm1,kkp1)
02910 - VAT3( uSW, ip1,jm1,kp1) * VAT3( oPC, ii,jjm1,kkp1)
02911 - VAT3( oE, i,jm1,kp1) * VAT3( dPN, ii,jjm1,kkp1)
02912 - VAT3( uW, ip1,jm1,kp1) * VAT3( oPN, ii,jjm1,kkp1)
02913 - VAT3( oN, ip1,jm2,kp1) * VAT3( dPE, ii,jjm1,kkp1)
02914 - VAT3( uS, ip1,jm1,kp1) * VAT3( oPE, ii,jjm1,kkp1)
02915 + VAT3( oC, ip1,jm1,kp1) * VAT3( dPNE, ii,jjm1,kkp1)
02916 - VAT3( uC, ip1,jm1,kp1) * VAT3( oPNE, ii,jjm1,kkp1));
02917
02918 TMP6_XUS =
02919 - VAT3( oPE, ii,jj,kk) * (- VAT3( uSW, ip1,j,k) * VAT3( dPN, ii,jjm1,kkp1)
02920 - VAT3( uS, ip1,j,k) * VAT3( dPNE, ii,jjm1,kkp1))
02921
02922 - VAT3( uPE, ii,jj,kk) * (- VAT3( oNE, i,jm1,kp1) * VAT3( dPN, ii,jjm1,kkp1)
02923 - VAT3( uSW, ip1,j,kp1) * VAT3( oPN, ii,jjm1,kkp1)
02924 - VAT3( oN, ip1,jm1,kp1) * VAT3( dPNE, ii,jjm1,kkp1)
02925 - VAT3( uS, ip1,j,kp1) * VAT3( oPNE, ii,jjm1,kkp1));
02926
02927 VAT3( XuS, ii,jj,kk) = TMP1_XUS + TMP2_XUS + TMP3_XUS + TMP4_XUS
02928 + TMP5_XUS + TMP6_XUS;
02929
02930 //fprintf(data, "%19.12E\n", VAT3(XuS, ii, jj, kk));
02931
02932 /* *****
02933 * *** > UNE;
02934 * *****
02935 // VAT3(XuNE, ii,jj,kk) =
02936 TMP1_XUNE =
02937 VAT3( oPC, ii,jj,kk) * VAT3( uNE, i,j,k) * VAT3( dPSW, iip1,jjp1,kkp1)
02938
02939 - VAT3( uPC, ii,jj,kk) * (- VAT3( oNE, i,j,kp1) * VAT3( dPSW, iip1,jjp1,kkp1)
02940 - VAT3( uNE, i,j,kp1) * VAT3( oPSW, iip1,jjp1,kkp1))
02941
02942 - VAT3( oPN, ii,jj,kk) * (- VAT3( uE, i,jp1,k) * VAT3( dPSW, iip1,jjp1,kkp1)
02943 - VAT3( uNE, i,jp1,k) * VAT3( dPW, iip1,jjp1,kkp1))
02944
02945 - VAT3( uPN, ii,jj,kk) * (- VAT3( oE, i,jp1,kp1) * VAT3( dPSW, iip1,jjp1,kkp1)
02946 - VAT3( uE, i,jp1,kp1) * VAT3( oPSW, iip1,jjp1,kkp1)
02947 - VAT3( oNE, i,jp1,kp1) * VAT3( dPW, iip1,jjp1,kkp1)
02948 - VAT3( uNE, i,jp1,kp1) * VAT3( oPW, iip1,jjp1,kkp1))
02949

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02950     - VAT3( oPE, ii,jj,kk) * (- VAT3( uN, ip1,j,k) * VAT3(dPSW, iip1,jjp1,kkp1)
02951       - VAT3( uNE, ip1,j,k) * VAT3( dPS, iip1,jjp1,kkp1));
02952
02953 TMP2_XUNE =
02954     - VAT3( uPE, ii,jj,kk) * (- VAT3( oN, ip1,j,kp1) * VAT3(dPSW, iip1,jjp1,kkp1)
02955       - VAT3( uN, ip1,j,kp1) * VAT3(oPSW, iip1,jjp1,kkp1)
02956       - VAT3( oNE, ip1,j,kp1) * VAT3( dPS, iip1,jjp1,kkp1)
02957       - VAT3( uNE, ip1,j,kp1) * VAT3( oPS, iip1,jjp1,kkp1))
02958
02959     - VAT3(oPNE, ii,jj,kk) * (- VAT3( uC, ip1,jp1,k) * VAT3(dPSW, iip1,jjp1,kkp1)
02960       - VAT3( uN, ip1,jp1,k) * VAT3( dPW, iip1,jjp1,kkp1)
02961       - VAT3( uE, ip1,jp1,k) * VAT3( dPS, iip1,jjp1,kkp1)
02962       - VAT3( uNE, ip1,jp1,k) * VAT3( dPC, iip1,jjp1,kkp1))
02963
02964     - VAT3(uPNE, ii,jj,kk) * ( VAT3( oC, ip1,jp1,kp1) * VAT3(dPSW, iip1,jjp1,kkp1)
02965       - VAT3( uC, ip1,jp1,kp1) * VAT3(oPSW, iip1,jjp1,kkp1)
02966       - VAT3( oN, ip1,jp1,kp1) * VAT3( dPW, iip1,jjp1,kkp1)
02967       - VAT3( uN, ip1,jp1,kp1) * VAT3( oPW, iip1,jjp1,kkp1)
02968       - VAT3( oE, ip1,jp1,kp1) * VAT3( dPS, iip1,jjp1,kkp1)
02969       - VAT3( uE, ip1,jp1,kp1) * VAT3( oPS, iip1,jjp1,kkp1)
02970       - VAT3( oNE, ip1,jp1,kp1) * VAT3( dPC, iip1,jjp1,kkp1)
02971       - VAT3( uNE, ip1,jp1,kp1) * VAT3( oPC, iip1,jjp1,kkp1));
02972 VAT3(XuNE, ii,jj,kk) = TMP1_XUNE + TMP2_XUNE;
02973
02974     //fprintf(data, "%19.12E\n", VAT3(XuNE, ii, jj, kk));
02975
02976     /* *****
02977      * *** > UNW;
02978      * *****/
02979
02980     // VAT3(XuNW, ii,jj,kk) =
02981 TMP1_XUNW =
02982     - VAT3( oPW, ii,jj,kk) * (- VAT3( uNW, im1,j,k) * VAT3( dPS, iim1,jjp1,kkp1)
02983       - VAT3( uN, im1,j,k) * VAT3(dPSE, iim1,jjp1,kkp1))
02984
02985     - VAT3( uPW, ii,jj,kk) * (- VAT3( oNW, im1,j,kp1) * VAT3( dPS, iim1,jjp1,kkp1)
02986       - VAT3( uNW, im1,j,kp1) * VAT3( oPS, iim1,jjp1,kkp1)
02987       - VAT3( oN, im1,j,kp1) * VAT3(dPSE, iim1,jjp1,kkp1)
02988       - VAT3( uN, im1,j,kp1) * VAT3(oPSE, iim1,jjp1,kkp1))
02989
02990     - VAT3(oPNW, ii,jj,kk) * (- VAT3( uW, im1,jp1,k) * VAT3( dPS, iim1,jjp1,kkp1)
02991       - VAT3( uNW, im1,jp1,k) * VAT3( dPC, iim1,jjp1,kkp1)
02992       - VAT3( uC, im1,jp1,k) * VAT3(dPSE, iim1,jjp1,kkp1)
02993       - VAT3( uN, im1,jp1,k) * VAT3( dPE, iim1,jjp1,kkp1));
02994
02995 TMP2_XUNW =
02996     - VAT3(uPNW, ii,jj,kk) * (- VAT3( oE, im2,jp1,kp1) * VAT3( dPS, iim1,jjp1,kkp1)
02997       - VAT3( uW, im1,jp1,kp1) * VAT3( oPS, iim1,jjp1,kkp1)
02998       - VAT3( oNW, im1,jp1,kp1) * VAT3( dPC, iim1,jjp1,kkp1)
02999       - VAT3( uNW, im1,jp1,kp1) * VAT3( oPC, iim1,jjp1,kkp1)
03000       + VAT3( oC, im1,jp1,kp1) * VAT3(dPSE, iim1,jjp1,kkp1)
03001       - VAT3( uC, im1,jp1,kp1) * VAT3(oPSE, iim1,jjp1,kkp1)
03002       - VAT3( oN, im1,jp1,kp1) * VAT3( dPE, iim1,jjp1,kkp1)
03003       - VAT3( uN, im1,jp1,kp1) * VAT3( oPE, iim1,jjp1,kkp1))
03004
03005     + VAT3( oPC, ii,jj,kk) * VAT3( uNW, i,j,k) * VAT3(dPSE, iim1,jjp1,kkp1)
03006
03007     - VAT3( uPC, ii,jj,kk) * (- VAT3( oNW, i,j,kp1) * VAT3(dPSE, iim1,jjp1,kkp1)
03008       - VAT3( uNW, i,j,kp1) * VAT3(oPSE, iim1,jjp1,kkp1))
03009
03010     - VAT3( oPN, ii,jj,kk) * (- VAT3( uW, i,jp1,k) * VAT3(dPSE, iim1,jjp1,kkp1)
03011       - VAT3( uNW, i,jp1,k) * VAT3( dPE, iim1,jjp1,kkp1))
03012
03013     - VAT3( uPN, ii,jj,kk) * (- VAT3( oE, im1,jp1,kp1) * VAT3(dPSE, iim1,jjp1,kkp1)
03014       - VAT3( uW, i,jp1,kp1) * VAT3(oPSE, iim1,jjp1,kkp1)
03015       - VAT3( oNW, i,jp1,kp1) * VAT3( dPE, iim1,jjp1,kkp1)
03016       - VAT3( uNW, i,jp1,kp1) * VAT3( oPE, iim1,jjp1,kkp1));
03017
03018 VAT3(XuNW, ii,jj,kk) = TMP1_XUNW + TMP2_XUNW;
03019
03020     //fprintf(data, "%19.12E\n", VAT3(XuNW, ii, jj, kk));
03021
03022     /* *****
03023      * *** > USE;
03024      * *****/
03025
03026     // VAT3(XuSE, ii,jj,kk) =
03027 TMP1_XUSE =
03028     - VAT3( oPS, ii,jj,kk) * (- VAT3( uSE, i,jm1,k) * VAT3( dPW, iip1,jjm1,kkp1)
03029       - VAT3( uE, i,jm1,k) * VAT3(dPNW, iip1,jjm1,kkp1))
03030

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03031      - VAT3( uPS, ii,jj,kk) * (- VAT3( oNW, ip1,jm2,kp1) * VAT3( dPW, iip1,jjml,kkp1)
03032      - VAT3( uSE, i, jml,kp1) * VAT3( oPW, iip1,jjml,kkp1)
03033      - VAT3( oE, i, jml,kp1) * VAT3(dPNW, iip1,jjml,kkp1)
03034      - VAT3( uE, i, jml,kp1) * VAT3(oPNW, iip1,jjml,kkp1))
03035
03036      + VAT3( oPC, ii,jj,kk) * VAT3( uSE, i, j, k) * VAT3(dPNW, iip1,jjml,kkp1)
03037
03038      - VAT3( uPC, ii,jj,kk) * (- VAT3( oNW, ip1,jml,kp1) * VAT3(dPNW, iip1,jjml,kkp1)
03039      - VAT3( uSE, i, j, kp1) * VAT3(oPNW, iip1,jjml,kkp1));
03040
03041      TMP2_XUSE =
03042      - VAT3(oPSE, ii,jj,kk) * (- VAT3( uS, ip1,jml,k) * VAT3( dPW, iip1,jjml,kkp1)
03043      - VAT3( uC, ip1,jml,k) * VAT3(dPNW, iip1,jjml,kkp1)
03044      - VAT3( uSE, ip1,jml,k) * VAT3( dPC, iip1,jjml,kkp1)
03045      - VAT3( uE, ip1,jml,k) * VAT3( dPN, iip1,jjml,kkp1))
03046
03047      - VAT3(uPSE, ii,jj,kk) * (- VAT3( oN, ip1,jm2,kp1) * VAT3( dPW, iip1,jjml,kkp1)
03048      - VAT3( uS, ip1,jml,kp1) * VAT3( oPW, iip1,jjml,kkp1)
03049      + VAT3( oC, ip1,jml,kp1) * VAT3(dPNW, iip1,jjml,kkp1)
03050      - VAT3( uC, ip1,jml,kp1) * VAT3(oPNW, iip1,jjml,kkp1)
03051      - VAT3( oNW, ip2,jm2,kp1) * VAT3( dPC, iip1,jjml,kkp1)
03052      - VAT3( uSE, ip1,jml,kp1) * VAT3( oPC, iip1,jjml,kkp1)
03053      - VAT3( oE, ip1,jml,kp1) * VAT3( dPN, iip1,jjml,kkp1)
03054      - VAT3( uE, ip1,jml,kp1) * VAT3( oPN, iip1,jjml,kkp1))
03055
03056      - VAT3( oPE, ii,jj,kk) * (- VAT3( uS, ip1,j,k) * VAT3(dPNW, iip1,jjml,kkp1)
03057      - VAT3( uSE, ip1,j,k) * VAT3( dPN, iip1,jjml,kkp1))
03058
03059      - VAT3( uPE, ii,jj,kk) * (- VAT3( oN, ip1,jml,kp1) * VAT3(dPNW, iip1,jjml,kkp1)
03060      - VAT3( uS, ip1,j,kp1) * VAT3(oPNW, iip1,jjml,kkp1)
03061      - VAT3( oNW, ip2,jml,kp1) * VAT3( dPN, iip1,jjml,kkp1)
03062      - VAT3( uSE, ip1,j,kp1) * VAT3( oPN, iip1,jjml,kkp1));
03063      VAT3(XuSE, ii,jj,kk) = TMP1_XUSE + TMP2_XUSE;
03064
03065      //fprintf(data, "%19.12E\n", VAT3(XuSE, ii, jj, kk));
03066
03067      /* *****
03068      * *** > USW;
03069      * *****/
03070
03071      // VAT3(XuSW, ii,jj,kk) =
03072      TMP1_XUSW =
03073      - VAT3(oPSW, ii,jj,kk) * (- VAT3( uSW, im1,jml,k) * VAT3( dPC, iim1,jjml,kkp1)
03074      - VAT3( uW, im1,jml,k) * VAT3( dPN, iim1,jjml,kkp1)
03075      - VAT3( uS, im1,jml,k) * VAT3( dPE, iim1,jjml,kkp1)
03076      - VAT3( uC, im1,jml,k) * VAT3(dPNE, iim1,jjml,kkp1))
03077
03078      - VAT3(uPSW, ii,jj,kk) * (- VAT3( oNE, im2,jm2,kp1) * VAT3( dPC, iim1,jjml,kkp1)
03079      - VAT3( uSW, im1,jml,kp1) * VAT3( oPC, iim1,jjml,kkp1)
03080      - VAT3( oE, im2,jml,kp1) * VAT3( dPN, iim1,jjml,kkp1)
03081      - VAT3( uW, im1,jml,kp1) * VAT3( oPN, iim1,jjml,kkp1)
03082      - VAT3( oN, im1,jm2,kp1) * VAT3( dPE, iim1,jjml,kkp1)
03083      - VAT3( uS, im1,jml,kp1) * VAT3( oPE, iim1,jjml,kkp1)
03084      + VAT3( oC, im1,jml,kp1) * VAT3(dPNE, iim1,jjml,kkp1)
03085      - VAT3( uC, im1,jml,kp1) * VAT3(oPNE, iim1,jjml,kkp1))
03086
03087      - VAT3( oPW, ii,jj,kk) * (- VAT3( uSW, im1,j,k) * VAT3( dPN, iim1,jjml,kkp1)
03088      - VAT3( uS, im1,j,k) * VAT3(dPNE, iim1,jjml,kkp1));
03089
03090      TMP2_XUSW =
03091      - VAT3( uPW, ii,jj,kk) * (- VAT3( oNE, im2,jml,kp1) * VAT3( dPN, iim1,jjml,kkp1)
03092      - VAT3( uSW, im1,j,kp1) * VAT3( oPN, iim1,jjml,kkp1)
03093      - VAT3( oN, im1,jml,kp1) * VAT3(dPNE, iim1,jjml,kkp1)
03094      - VAT3( uS, im1,j,kp1) * VAT3(oPNE, iim1,jjml,kkp1))
03095
03096      - VAT3( oPS, ii,jj,kk) * (- VAT3( uSW, i, jml,k) * VAT3( dPE, iim1,jjml,kkp1)
03097      - VAT3( uW, i, jml,k) * VAT3(dPNE, iim1,jjml,kkp1))
03098
03099      - VAT3( uPS, ii,jj,kk) * (- VAT3( oNE, im1,jm2,kp1) * VAT3( dPE, iim1,jjml,kkp1)
03100      - VAT3( uSW, i, jml,kp1) * VAT3( oPE, iim1,jjml,kkp1)
03101      - VAT3( oE, im1,jml,kp1) * VAT3(dPNE, iim1,jjml,kkp1)
03102      - VAT3( uW, i, jml,kp1) * VAT3(oPNE, iim1,jjml,kkp1))
03103
03104      + VAT3( oPC, ii,jj,kk) * VAT3( uSW, i, j, k) * VAT3(dPNE, iim1,jjml,kkp1)
03105
03106      - VAT3( uPC, ii,jj,kk) * (- VAT3( oNE, im1,jml,kp1) * VAT3(dPNE, iim1,jjml,kkp1)
03107      - VAT3( uSW, i, j, kp1) * VAT3(oPNE, iim1,jjml,kkp1));
03108      VAT3(XuSW, ii,jj,kk) = TMP1_XUSW + TMP2_XUSW;
03109
03110      //fprintf(data, "%19.12E\n", VAT3(XuSW, ii, jj, kk));
03111

```

```

03112     }
03113     }
03114 }
03115 }

```

9.119 buildGd.h

```

00001
00049 #ifndef _BUILGD_H_
00050 #define _BUILGD_H_
00051
00052 #include "malloc/malloc.h"
00053
00054 #include "apbscfg.h"
00055
00056 #include "generic/vhal.h"
00057 #include "generic/vmatrix.h"
00058
00059 VEXTERNC void VbuildG(
00060     int      *nxf,
00061     int      *nyf,
00062     int      *nzf,
00063     int      *nxc,
00064     int      *nyc,
00065     int      *nzc,
00066     int      *numdia,
00067     double   *pcFF,
00068     double   *acFF,
00069     double   *ac
00070 );
00071
00144 VEXTERNC void VbuildG_1(
00145     int      *nxf,
00146     int      *nyf,
00147     int      *nzf,
00148     int      *nx,
00149     int      *ny,
00150     int      *nz,
00151     double   *oPC,
00152     double   *oPN,
00153     double   *oPS,
00154     double   *oPE,
00155     double   *oPW,
00156     double   *oPNE,
00157     double   *oPNW,
00158     double   *oPSE,
00159     double   *oPSW,
00160     double   *uPC,
00161     double   *uPN,
00162     double   *uPS,
00163     double   *uPE,
00164     double   *uPW,
00165     double   *uPNE,
00166     double   *uPNW,
00167     double   *uPSE,
00168     double   *uPSW,
00169     double   *dPC,
00170     double   *dPN,
00171     double   *dPS,
00172     double   *dPE,
00173     double   *dPW,
00174     double   *dPNE,
00175     double   *dPNW,
00176     double   *dPSE,
00177     double   *dPSW,
00178     double   *oC,
00179     double   *XoC,
00180     double   *XoE,
00181     double   *XoN,
00182     double   *XuC,
00183     double   *XoNE,
00184     double   *XoNW,
00185     double   *XuE,
00186     double   *XuW,
00187     double   *XuN,
00188     double   *XuS,
00189     double   *XuNE,
00190     double   *XuNW,

```

```
00191         double *XuSE,
00192         double *XuSW
00193     );
00194
00195
00196
00276 VEXTERNC void VbuildG_7(
00277     int     *nxf,
00278     int     *nyf,
00279     int     *nzf,
00280     int     *nx,
00281     int     *ny,
00282     int     *nz,
00283     double  *oPC,
00284     double  *oPN,
00285     double  *oPS,
00286     double  *oPE,
00287     double  *oPW,
00288     double  *oPNE,
00289     double  *oPNW,
00290     double  *oPSE,
00291     double  *oPSW,
00292     double  *uPC,
00293     double  *uPN,
00294     double  *uPS,
00295     double  *uPE,
00296     double  *uPW,
00297     double  *uPNE,
00298     double  *uPNW,
00299     double  *uPSE,
00300     double  *uPSW,
00301     double  *dPC,
00302     double  *dPN,
00303     double  *dPS,
00304     double  *dPE,
00305     double  *dPW,
00306     double  *dPNE,
00307     double  *dPNW,
00308     double  *dPSE,
00309     double  *dPSW,
00310     double  *oC,
00311     double  *oE,
00312     double  *oN,
00313     double  *uC,
00314     double  *XoC,
00315     double  *XoE,
00316     double  *XoN,
00317     double  *XuC,
00318     double  *XoNE,
00319     double  *XoNW,
00320     double  *XuE,
00321     double  *XuW,
00322     double  *XuN,
00323     double  *XuS,
00324     double  *XuNE,
00325     double  *XuNW,
00326     double  *XuSE,
00327     double  *XuSW
00328 );
00329
00330
00423 VEXTERNC void VbuildG_27(
00424     int     *nxf,
00425     int     *nyf,
00426     int     *nzf,
00427     int     *nx,
00428     int     *ny,
00429     int     *nz,
00430     double  *oPC,
00431     double  *oPN,
00432     double  *oPS,
00433     double  *oPE,
00434     double  *oPW,
00435     double  *oPNE,
00436     double  *oPNW,
00437     double  *oPSE,
00438     double  *oPSW,
00439     double  *uPC,
00440     double  *uPN,
00441     double  *uPS,
00442     double  *uPE,
```

```

00443         double *uPW,
00444         double *uPNE,
00445         double *uPNW,
00446         double *uPSE,
00447         double *uPSW,
00448         double *dPC,
00449         double *dPN,
00450         double *dPS,
00451         double *dPE,
00452         double *dPW,
00453         double *dPNE,
00454         double *dPNW,
00455         double *dPSE,
00456         double *dPSW,
00457         double *oC,
00458         double *oE,
00459         double *oN,
00460         double *uC,
00461         double *oNE,
00462         double *oNW,
00463         double *uE,
00464         double *uW,
00465         double *uN,
00466         double *uS,
00467         double *uNE,
00468         double *uNW,
00469         double *uSE,
00470         double *uSW,
00471         double *XoC,
00472         double *XoE,
00473         double *XoN,
00474         double *XuC,
00475         double *XoNE,
00476         double *XoNW,
00477         double *XuE,
00478         double *XuW,
00479         double *XuN,
00480         double *XuS,
00481         double *XuNE,
00482         double *XuNW,
00483         double *XuSE,
00484         double *XuSW
00485     );
00486
00487 #endif // _BUILDDGD_H_

```

9.120 buildPd.c

```

00001
00055 #include "buildPd.h"
00056
00057 VPUBLIC void VbuildP(int *nxf, int *nyf, int *nzf,
00058                     int *nxc, int *nyc, int *nzc,
00059                     int *mgprol,
00060                     int *ipc, double *rpc,
00061                     double *pc, double *ac,
00062                     double *xf, double *yf, double *zf) {
00063
00064     int numdia;
00065
00066     MAT2(pc, *nxc * *nyc * *nzc, 1);
00067     MAT2(ac, *nxf * *nyf * *nzf, 1);
00068
00069     if (*mgprol == 0) {
00070
00071         VbuildP_trilin(nxf, nyf, nzf,
00072                       nxc, nyc, nzc,
00073                       RAT2(pc, 1, 1),
00074                       xf, yf, zf);
00075
00076     } else if (*mgprol == 1) {
00077
00078         numdia = VAT(ipc, 11);
00079
00080         if (numdia == 7) {
00081             VbuildP_op7(nxf, nyf, nzf,
00082                       nxc, nyc, nzc,
00083                       ipc, rpc,

```

```

00084         RAT2(ac, 1, 1), RAT2(pc, 1, 1));
00085     } else if (numdia == 27) {
00086         VbuildP_op27(nxf, nyf, nzf,
00087             nxc, nyc, nzc,
00088             ipc, rpc,
00089             RAT2(ac, 1, 1), RAT2(pc, 1, 1));
00090     } else {
00091         Vnm_print(2,"BUILDP: invalid stencil type given: %d\n", numdia);
00092     }
00093 }
00094 }
00095
00096 VPUBLIC void VbuildP_trilin(int *nxf, int *nyf, int *nzf,
00097     int *nxc, int *nyc, int *nzc,
00098     double *pc,
00099     double *xf, double *yf, double *zf) {
00100
00101     MAT2(pc, *nxc * *nyc * *nzc, 1);
00102
00103     VbuildPb_trilin(nxf, nyf, nzf,
00104         nxc, nyc, nzc,
00105         RAT2(pc, 1, 1),RAT2(pc, 1, 2),RAT2(pc, 1, 3),RAT2(pc, 1, 4),RAT2(pc, 1, 5),
00106         RAT2(pc, 1, 6),RAT2(pc, 1, 7),RAT2(pc, 1, 8),RAT2(pc, 1, 9),
00107         RAT2(pc, 1, 10),RAT2(pc, 1, 11),RAT2(pc, 1, 12),RAT2(pc, 1, 13),RAT2(pc, 1, 14),
00108         RAT2(pc, 1, 15),RAT2(pc, 1, 16),RAT2(pc, 1, 17),RAT2(pc, 1, 18),
00109         RAT2(pc, 1, 19),RAT2(pc, 1, 20),RAT2(pc, 1, 21),RAT2(pc, 1, 22),RAT2(pc, 1, 23),
00110         RAT2(pc, 1, 24),RAT2(pc, 1, 25),RAT2(pc, 1, 26),RAT2(pc, 1, 27),
00111         xf, yf, zf);
00112 }
00113
00114 VEXTERNC void VbuildPb_trilin(int *nxf, int *nyf, int *nzf,
00115     int *nxc, int *nyc, int *nzc,
00116     double *oPC, double *oPN, double *oPS, double *oPE, double *oPW,
00117     double *oPNE, double *oPNW, double *oPSE, double *oPSW,
00118     double *uPC, double *uPN, double *uPS, double *uPE, double *uPW,
00119     double *uPNE, double *uPNW, double *uPSE, double *uPSW,
00120     double *dPC, double *dPN, double *dPS, double *dPE, double *dPW,
00121     double *dPNE, double *dPNW, double *dPSE, double *dPSW,
00122     double *xf, double *yf, double *zf) {
00123
00124     int i, j, k;
00125
00126
00127     double won      = 1.0;
00128     double half     = 1.0 / 2.0;
00129     double quarter  = 1.0 / 4.0;
00130     double eighth   = 1.0 / 8.0;
00131
00132     MAT3( oPC, *nxc, *nyc, *nzc);
00133     MAT3( oPN, *nxc, *nyc, *nzc);
00134     MAT3( oPS, *nxc, *nyc, *nzc);
00135     MAT3( oPE, *nxc, *nyc, *nzc);
00136     MAT3( oPW, *nxc, *nyc, *nzc);
00137
00138     MAT3(oPNE, *nxc, *nyc, *nzc);
00139     MAT3(oPNW, *nxc, *nyc, *nzc);
00140     MAT3(oPSE, *nxc, *nyc, *nzc);
00141     MAT3(oPSW, *nxc, *nyc, *nzc);
00142
00143     MAT3( uPC, *nxc, *nyc, *nzc);
00144     MAT3( uPN, *nxc, *nyc, *nzc);
00145     MAT3( uPS, *nxc, *nyc, *nzc);
00146     MAT3( uPE, *nxc, *nyc, *nzc);
00147     MAT3( uPW, *nxc, *nyc, *nzc);
00148
00149     MAT3(uPNE, *nxc, *nyc, *nzc);
00150     MAT3(uPNW, *nxc, *nyc, *nzc);
00151     MAT3(uPSE, *nxc, *nyc, *nzc);
00152     MAT3(uPSW, *nxc, *nyc, *nzc);
00153
00154     MAT3( dPC, *nxc, *nyc, *nzc);
00155     MAT3( dPN, *nxc, *nyc, *nzc);
00156     MAT3( dPS, *nxc, *nyc, *nzc);
00157     MAT3( dPE, *nxc, *nyc, *nzc);
00158     MAT3( dPW, *nxc, *nyc, *nzc);
00159
00160     MAT3(dPNE, *nxc, *nyc, *nzc);
00161     MAT3(dPNW, *nxc, *nyc, *nzc);
00162     MAT3(dPSE, *nxc, *nyc, *nzc);
00163     MAT3(dPSW, *nxc, *nyc, *nzc);
00164
00165     for(k=2; k<=*nzc-1; k++) {

```



```

00166     for(j=2; j<=*nyc-1; j++) {
00167         for(i=2; i<=*nxc-1; i++) {
00168
00169             VAT3(oPC, i,j,k)  = won;
00170
00171             VAT3(oPN, i,j,k)  = half;
00172             VAT3(oPS, i,j,k)  = half;
00173             VAT3(oPE, i,j,k)  = half;
00174             VAT3(oPW, i,j,k)  = half;
00175             VAT3(uPC, i,j,k)  = half;
00176             VAT3(dPC, i,j,k)  = half;
00177
00178             VAT3(oPNE, i,j,k) = quarter;
00179             VAT3(oPNW, i,j,k) = quarter;
00180             VAT3(oPSE, i,j,k) = quarter;
00181             VAT3(oPSW, i,j,k) = quarter;
00182             VAT3(dPN, i,j,k)  = quarter;
00183             VAT3(dPS, i,j,k)  = quarter;
00184             VAT3(dPE, i,j,k)  = quarter;
00185             VAT3(dPW, i,j,k)  = quarter;
00186             VAT3(uPN, i,j,k)  = quarter;
00187             VAT3(uPS, i,j,k)  = quarter;
00188             VAT3(uPE, i,j,k)  = quarter;
00189             VAT3(uPW, i,j,k)  = quarter;
00190
00191             VAT3(dPNE, i,j,k) = eighth;
00192             VAT3(dPNW, i,j,k) = eighth;
00193             VAT3(dPSE, i,j,k) = eighth;
00194             VAT3(dPSW, i,j,k) = eighth;
00195             VAT3(uPNE, i,j,k) = eighth;
00196             VAT3(uPNW, i,j,k) = eighth;
00197             VAT3(uPSE, i,j,k) = eighth;
00198             VAT3(uPSW, i,j,k) = eighth;
00199         }
00200     }
00201 }
00202 }
00203
00204
00205
00206 VPUBLIC void VbuildP_op7(int *nxf, int *nyf, int *nzf,
00207     int *nxc, int *nyc, int *nzc,
00208     int *ipc, double *rpc,
00209     double *ac, double *pc) {
00210
00211     MAT2(ac, *nxf * *nyf * *nzf, 1);
00212     MAT2(pc, *nxc * *nyc * *nzc, 1);
00213
00214     WARN_UNTESTED;
00215
00216     VbuildPb_op7(nxf, nyf, nzf,
00217         nxc, nyc, nzc,
00218         ipc, rpc,
00219         RAT2(ac, 1, 1), RAT2(ac, 1, 2), RAT2(ac, 1, 3),
00220         RAT2(ac, 1, 4),
00221         RAT2(pc, 1, 1), RAT2(pc, 1, 2), RAT2(pc, 1, 3), RAT2(pc, 1, 4), RAT2(pc, 1, 5),
00222         RAT2(pc, 1, 6), RAT2(pc, 1, 7), RAT2(pc, 1, 8), RAT2(pc, 1, 9),
00223         RAT2(pc, 1, 10), RAT2(pc, 1, 11), RAT2(pc, 1, 12), RAT2(pc, 1, 13), RAT2(pc, 1, 14),
00224         RAT2(pc, 1, 15), RAT2(pc, 1, 16), RAT2(pc, 1, 17), RAT2(pc, 1, 18),
00225         RAT2(pc, 1, 19), RAT2(pc, 1, 20), RAT2(pc, 1, 21), RAT2(pc, 1, 22), RAT2(pc, 1, 23),
00226         RAT2(pc, 1, 24), RAT2(pc, 1, 25), RAT2(pc, 1, 26), RAT2(pc, 1, 27));
00227 }
00228
00229
00230
00231 VPUBLIC void VbuildPb_op7(int *nxf, int *nyf, int *nzf,
00232     int *nxc, int *nyc, int *nzc,
00233     int *ipc, double *rpc,
00234     double *oC, double *oE, double *oN,
00235     double *uC,
00236     double *oPC, double *oPN, double *oPS, double *oPE, double *oPW,
00237     double *oPNE, double *oPNW, double *oPSE, double *oPSW,
00238     double *uPC, double *uPN, double *uPS, double *uPE, double *uPW,
00239     double *uPNE, double *uPNW, double *uPSE, double *uPSW,
00240     double *dPC, double *dPN, double *dPS, double *dPE, double *dPW,
00241     double *dPNE, double *dPNW, double *dPSE, double *dPSW) {
00242
00243     int i, j, k;
00244     int ii, jj, kk;
00245     int im1, ip1;
00246     int im2, ip2;

```

```

00247     int  jml,  jpl;
00248     int  jm2,  jp2;
00249     int  km1,  kpl;
00250     int  km2,  kp2;
00251     int  iim1, iip1;
00252     int  jjm1, jjp1;
00253     int  kkm1, kkpl;
00254
00255     double won, half, quarter, eighth;
00256
00257     MAT3( oC, *nxf, *nyf, *nzf);
00258     MAT3( oE, *nxf, *nyf, *nzf);
00259     MAT3( oN, *nxf, *nyf, *nzf);
00260     MAT3( uC, *nxf, *nyf, *nzf);
00261     MAT3( oPC, *nxc, *nyc, *nzc);
00262     MAT3( oPN, *nxc, *nyc, *nzc);
00263     MAT3( oPS, *nxc, *nyc, *nzc);
00264     MAT3( oPE, *nxc, *nyc, *nzc);
00265     MAT3( oPW, *nxc, *nyc, *nzc);
00266     MAT3( oPNE, *nxc, *nyc, *nzc);
00267     MAT3( oPNW, *nxc, *nyc, *nzc);
00268     MAT3( oPSE, *nxc, *nyc, *nzc);
00269     MAT3( oPSW, *nxc, *nyc, *nzc);
00270     MAT3( uPC, *nxc, *nyc, *nzc);
00271     MAT3( uPN, *nxc, *nyc, *nzc);
00272     MAT3( uPS, *nxc, *nyc, *nzc);
00273     MAT3( uPE, *nxc, *nyc, *nzc);
00274     MAT3( uPW, *nxc, *nyc, *nzc);
00275     MAT3( uPNE, *nxc, *nyc, *nzc);
00276     MAT3( uPNW, *nxc, *nyc, *nzc);
00277     MAT3( uPSE, *nxc, *nyc, *nzc);
00278     MAT3( uPSW, *nxc, *nyc, *nzc);
00279     MAT3( dPC, *nxc, *nyc, *nzc);
00280     MAT3( dPN, *nxc, *nyc, *nzc);
00281     MAT3( dPS, *nxc, *nyc, *nzc);
00282     MAT3( dPE, *nxc, *nyc, *nzc);
00283     MAT3( dPW, *nxc, *nyc, *nzc);
00284     MAT3( dPNE, *nxc, *nyc, *nzc);
00285     MAT3( dPNW, *nxc, *nyc, *nzc);
00286     MAT3( dPSE, *nxc, *nyc, *nzc);
00287     MAT3( dPSW, *nxc, *nyc, *nzc);
00288
00289     WARN_UNTESTED;
00290
00291     // interpolation stencil ***
00292     won    = 1.0;
00293     half   = 1.0 / 2.0;
00294     quarter = 1.0 / 4.0;
00295     eighth = 1.0 / 8.0;
00296
00297     //fprintf(data, "%s\n", PRINT_FUNC);
00298
00299     for (kk = 2; kk < *nzc - 1; kk++) {
00300         k = 2 * kk - 1;
00301
00302         for (jj = 2; jj < *nyc - 1; jj++) {
00303             j = 2 * jj - 1;
00304
00305             for (ii = 2; ii < *nxc - 1; ii++) {
00306                 i = 2 * ii - 1;
00307
00308                 // index computations ***
00309                 im1 = i - 1;
00310                 ip1 = i + 1;
00311                 im2 = i - 2;
00312                 ip2 = i + 2;
00313                 jml = j - 1;
00314                 jpl = j + 1;
00315                 jm2 = j - 2;
00316                 jp2 = j + 2;
00317                 km1 = k - 1;
00318                 kpl = k + 1;
00319                 km2 = k - 2;
00320                 kp2 = k + 2;
00321                 iim1 = ii - 1;
00322                 iip1 = ii + 1;
00323                 jjm1 = jj - 1;
00324                 jjp1 = jj + 1;
00325                 kkm1 = kk - 1;
00326                 kkpl = kk + 1;
00327

```

```

00328 // *****
00329 // *** > oPC;
00330 // *****
00331
00332 VAT3( oPC, ii, jj, kk) = won;
00333
00334 //fprintf(data, "%19.12E\n", VAT3(oPC, ii, jj, kk));
00335
00336 // *****
00337 // *** > oPN;
00338 // *****
00339
00340 VAT3( oPN, ii, jj, kk) =
00341     VAT3( oN, i, j, k) / ( VAT3( oC, i, jpl, k)
00342         - VAT3( oE, iml, jpl, k)
00343         - VAT3( oE, i, jpl, k)
00344         - VAT3( uC, i, jpl, kml)
00345         - VAT3( uC, i, jpl, k));
00346
00347 //fprintf(data, "%19.12E\n", VAT3(oPN, ii, jj, kk));
00348
00349 // *****
00350 // *** > oPS;
00351 // *****
00352
00353 VAT3( oPS, ii, jj, kk) =
00354     VAT3( oN, i, jml, k) / ( VAT3( oC, i, jml, k)
00355         - VAT3( oE, iml, jml, k)
00356         - VAT3( oE, i, jml, k)
00357         - VAT3( uC, i, jml, kml)
00358         - VAT3( uC, i, jml, k));
00359
00360 //fprintf(data, "%19.12E\n", VAT3(oPS, ii, jj, kk));
00361
00362 // *****
00363 // *** > oPE;
00364 // *****
00365
00366 VAT3( oPE, ii, jj, kk) =
00367     VAT3( oE, i, j, k) / ( VAT3( oC, ip1, j, k)
00368         - VAT3( uC, ip1, j, kml)
00369         - VAT3( uC, ip1, j, k)
00370         - VAT3( oN, ip1, j, k)
00371         - VAT3( oN, ip1, jml, k));
00372
00373 //fprintf(data, "%19.12E\n", VAT3(oPE, ii, jj, kk));
00374
00375 // *****
00376 // *** > oPW;
00377 // *****
00378
00379 VAT3( oPW, ii, jj, kk) =
00380     VAT3( oE, iml, j, k) / ( VAT3( oC, iml, j, k)
00381         - VAT3( uC, iml, j, kml)
00382         - VAT3( uC, iml, j, k)
00383         - VAT3( oN, iml, j, k)
00384         - VAT3( oN, iml, jml, k));
00385
00386 //fprintf(data, "%19.12E\n", VAT3(oPW, ii, jj, kk));
00387
00388 // *****
00389 // *** > oPNE;
00390 // *****
00391
00392 VAT3( oPNE, ii, jj, kk) =
00393     (
00394         VAT3( oN, ip1, j, k) * VAT3( oPE, ii, jj, kk)
00395         + VAT3( oE, i, jpl, k) * VAT3( oPN, ii, jj, kk)
00396     ) / (
00397         VAT3( oC, ip1, jpl, k)
00398         - VAT3( uC, ip1, jpl, kml)
00399         - VAT3( uC, ip1, jpl, k)
00400     );
00401
00402 //fprintf(data, "%19.12E\n", VAT3(oPNE, ii, jj, kk));
00403
00404 // *****
00405 // *** > oPNW;
00406 // *****
00407
00408 VAT3( oPNW, ii, jj, kk) =

```

```

00409      (
00410          VAT3( oN, iml, j, k) * VAT3( oPW, ii, jj, kk)
00411      + VAT3( oE, iml, jpl, k) * VAT3( oPN, ii, jj, kk)
00412      ) / (
00413          VAT3( oC, iml, jpl, k)
00414      - VAT3( uC, iml, jpl, kml)
00415      - VAT3( uC, iml, jpl, k)
00416      );
00417
00418      //fprintf(data, "%19.12E\n", VAT3(oPNW, ii, jj, kk));
00419
00420      // *****
00421      // *** > oPSE;
00422      // *****
00423
00424      VAT3(oPSE, ii, jj, kk) =
00425      (
00426          VAT3( oN, ip1, jml, k) * VAT3( oPE, ii, jj, kk)
00427      + VAT3( oE, i, jml, k) * VAT3( oPS, ii, jj, kk)
00428      ) / (
00429          VAT3( oC, ip1, jml, k)
00430      - VAT3( uC, ip1, jml, kml)
00431      - VAT3( uC, ip1, jml, k)
00432      );
00433
00434      //fprintf(data, "%19.12E\n", VAT3(oPSE, ii, jj, kk));
00435
00436      // *****
00437      // *** > oPSW;
00438      // *****
00439
00440      VAT3(oPSW, ii, jj, kk) =
00441      (
00442          VAT3( oN, iml, jml, k) * VAT3( oPW, ii, jj, kk)
00443      + VAT3( oE, iml, jml, k) * VAT3( oPS, ii, jj, kk)
00444      ) / (
00445          VAT3( oC, iml, jml, k)
00446      - VAT3( uC, iml, jml, kml)
00447      - VAT3( uC, iml, jml, k)
00448      );
00449
00450      //fprintf(data, "%19.12E\n", VAT3(oPSW, ii, jj, kk));
00451
00452      // *****
00453      // *** > dPC;
00454      // *****
00455
00456      VAT3( dPC, ii, jj, kk) =
00457          VAT3( uC, i, j, kml)
00458      / (
00459          VAT3( oC, i, j, kml)
00460      - VAT3( oN, i, j, kml)
00461      - VAT3( oN, i, jml, kml)
00462      - VAT3( oE, iml, j, kml)
00463      - VAT3( oE, i, j, kml)
00464      );
00465
00466      //fprintf(data, "%19.12E\n", VAT3(dPC, ii, jj, kk));
00467
00468      // *****
00469      // *** > dPN;
00470      // *****
00471
00472      VAT3( dPN, ii, jj, kk) =
00473      (
00474          VAT3( oN, i, j, kml) * VAT3( dPC, ii, jj, kk)
00475      + VAT3( uC, i, jpl, kml) * VAT3( oPN, ii, jj, kk)
00476      ) / (
00477          VAT3( oC, i, jpl, kml)
00478      - VAT3( oE, iml, jpl, kml)
00479      - VAT3( oE, i, jpl, kml)
00480      );
00481
00482      //fprintf(data, "%19.12E\n", VAT3(dPN, ii, jj, kk));
00483
00484      // *****
00485      // *** > dPS;
00486      // *****
00487
00488      VAT3( dPS, ii, jj, kk) =
00489      (

```

```

00490          VAT3( oN, i, jml, kml) * VAT3( dPC, ii, jj, kk)
00491      + VAT3( uC, i, jml, kml) * VAT3( oPS, ii, jj, kk)
00492      ) / (
00493          VAT3( oC, i, jml, kml)
00494      - VAT3( oE, iml, jml, kml)
00495      - VAT3( oE, i, jml, kml)
00496      );
00497
00498      //fprintf(data, "%19.12E\n", VAT3(dPS, ii, jj, kk));
00499
00500      // *****
00501      // *** > dPE;
00502      // *****
00503
00504      VAT3( dPE, ii, jj, kk) =
00505      (
00506          VAT3( uC, ip1, j, kml) * VAT3( oPE, ii, jj, kk)
00507      + VAT3( oE, i, j, kml) * VAT3( dPC, ii, jj, kk)
00508      ) / (
00509          VAT3( oC, ip1, j, kml)
00510      - VAT3( oN, ip1, j, kml)
00511      - VAT3( oN, ip1, jml, kml)
00512      );
00513
00514      //fprintf(data, "%19.12E\n", VAT3(dPE, ii, jj, kk));
00515
00516      // *****
00517      // *** > dPW;
00518      // *****
00519
00520      VAT3( dPW, ii, jj, kk) =
00521      (
00522          VAT3( uC, iml, j, kml) * VAT3( oPW, ii, jj, kk)
00523      + VAT3( oE, iml, j, kml) * VAT3( dPC, ii, jj, kk)
00524      ) / (
00525          VAT3( oC, iml, j, kml)
00526      - VAT3( oN, iml, j, kml)
00527      - VAT3( oN, iml, jml, kml)
00528      );
00529
00530      //fprintf(data, "%19.12E\n", VAT3(dPW, ii, jj, kk));
00531
00532      // *****
00533      // *** > dPNE;
00534      // *****
00535
00536      VAT3( dPNE, ii, jj, kk) =
00537      (
00538          VAT3( uC, ip1, jp1, kml) * VAT3( oPNE, ii, jj, kk)
00539      + VAT3( oE, i, jp1, kml) * VAT3( dPN, ii, jj, kk)
00540      + VAT3( oN, ip1, j, kml) * VAT3( dPE, ii, jj, kk)
00541      ) / VAT3( oC, ip1, jp1, kml);
00542
00543      //fprintf(data, "%19.12E\n", VAT3(dPNE, ii, jj, kk));
00544
00545      // *****
00546      // *** > dPNW;
00547      // *****
00548
00549      VAT3( dPNW, ii, jj, kk) =
00550      (
00551          VAT3( uC, iml, jp1, kml) * VAT3( oPNW, ii, jj, kk)
00552      + VAT3( oE, iml, jp1, kml) * VAT3( dPN, ii, jj, kk)
00553      + VAT3( oN, iml, j, kml) * VAT3( dPW, ii, jj, kk)
00554      ) / VAT3( oC, iml, jp1, kml);
00555
00556      //fprintf(data, "%19.12E\n", VAT3(dPNW, ii, jj, kk));
00557
00558      // *****
00559      // *** > dPSE;
00560      // *****
00561
00562      VAT3( dPSE, ii, jj, kk) =
00563      (
00564          VAT3( uC, ip1, jml, kml) * VAT3( oPSE, ii, jj, kk)
00565      + VAT3( oE, i, jml, kml) * VAT3( dPS, ii, jj, kk)
00566      + VAT3( oN, ip1, jml, kml) * VAT3( dPE, ii, jj, kk)
00567      ) / VAT3( oC, ip1, jml, kml);
00568
00569      //fprintf(data, "%19.12E\n", VAT3(dPSE, ii, jj, kk));
00570

```

```

00571 // *****
00572 // *** > dPSW;
00573 // *****
00574
00575 VAT3(dPSW, ii, jj, kk) =
00576 (
00577     VAT3( uC, iml, jml, kml) * VAT3(oPSW, ii, jj, kk)
00578     + VAT3( oE, iml, jml, kml) * VAT3( dPS, ii, jj, kk)
00579     + VAT3( oN, iml, jml, kml) * VAT3( dPW, ii, jj, kk)
00580 ) / VAT3( oC, iml, jml, kml);
00581
00582 //fprintf(data, "%19.12E\n", VAT3(dPSW, ii, jj, kk));
00583
00584 // *****
00585 // *** > uPC;
00586 // *****
00587
00588 VAT3( uPC, ii, jj, kk) =
00589     VAT3( uC, i, j, k)
00590     / ( VAT3( oC, i, j, kpl)
00591         - VAT3( oN, i, j, kpl)
00592         - VAT3( oN, i, jml, kpl)
00593         - VAT3( oE, iml, j, kpl)
00594         - VAT3( oE, i, j, kpl)
00595     );
00596
00597 //fprintf(data, "%19.12E\n", VAT3(uPC, ii, jj, kk));
00598
00599 // *****
00600 // *** > uPN;
00601 // *****
00602
00603 VAT3( uPN, ii, jj, kk) =
00604 (
00605     VAT3( oN, i, j, kpl) * VAT3( uPC, ii, jj, kk)
00606     + VAT3( uC, i, jpl, k) * VAT3( oPN, ii, jj, kk)
00607 ) / (
00608     VAT3( oC, i, jpl, kpl)
00609     - VAT3( oE, iml, jpl, kpl)
00610     - VAT3( oE, i, jpl, kpl)
00611 );
00612
00613 //fprintf(data, "%19.12E\n", VAT3(uPN, ii, jj, kk));
00614
00615 // *****
00616 // *** > uPS;
00617 // *****
00618
00619 VAT3( uPS, ii, jj, kk) =
00620 (
00621     VAT3( oN, i, jml, kpl) * VAT3( uPC, ii, jj, kk)
00622     + VAT3( uC, i, jml, k) * VAT3( oPS, ii, jj, kk)
00623 ) / (
00624     VAT3( oC, i, jml, kpl)
00625     - VAT3( oE, iml, jml, kpl)
00626     - VAT3( oE, i, jml, kpl)
00627 );
00628
00629 //fprintf(data, "%19.12E\n", VAT3(uPS, ii, jj, kk));
00630
00631 // *****
00632 // *** > uPE;
00633 // *****
00634
00635 VAT3( uPE, ii, jj, kk) =
00636 (
00637     VAT3( uC, ip1, j, k) * VAT3( oPE, ii, jj, kk)
00638     + VAT3( oE, i, j, kpl) * VAT3( uPC, ii, jj, kk)
00639 ) / (
00640     VAT3( oC, ip1, j, kpl)
00641     - VAT3( oN, ip1, j, kpl)
00642     - VAT3( oN, ip1, jml, kpl)
00643 );
00644
00645 //fprintf(data, "%19.12E\n", VAT3(uPE, ii, jj, kk));
00646
00647 // *****
00648 // *** > uPW;
00649 // *****
00650
00651 VAT3( uPW, ii, jj, kk) =

```

```

00652         (
00653             VAT3( uC, iml, j, k) * VAT3( oPW, ii, jj, kk)
00654         + VAT3( oE, iml, j, kpl) * VAT3( uPC, ii, jj, kk)
00655         ) / (
00656             VAT3( oC, iml, j, kpl)
00657         - VAT3( oN, iml, j, kpl)
00658         - VAT3( oN, iml, jml, kpl)
00659         );
00660
00661         //fprintf(data, "%19.12E\n", VAT3(uPW, ii, jj, kk));
00662
00663         // *****
00664         // *** > uPNE;
00665         // *****
00666
00667         VAT3(uPNE, ii, jj, kk) =
00668         (
00669             VAT3( uC, ip1, jpl, k) * VAT3(oPNE, ii, jj, kk)
00670         + VAT3( oE, i, jpl, kpl) * VAT3( uPN, ii, jj, kk)
00671         + VAT3( oN, ip1, j, kpl) * VAT3( uPE, ii, jj, kk)
00672         ) / VAT3( oC, ip1, jpl, kpl);
00673
00674         //fprintf(data, "%19.12E\n", VAT3(uPNE, ii, jj, kk));
00675
00676         // *****
00677         // *** > uPNW;
00678         // *****
00679
00680         VAT3(uPNW, ii, jj, kk) =
00681         (
00682             VAT3( uC, iml, jpl, k) * VAT3(oPNW, ii, jj, kk)
00683         + VAT3( oE, iml, jpl, kpl) * VAT3( uPN, ii, jj, kk)
00684         + VAT3( oN, iml, j, kpl) * VAT3( uPW, ii, jj, kk)
00685         ) / VAT3( oC, iml, jpl, kpl);
00686
00687         //fprintf(data, "%19.12E\n", VAT3(uPNW, ii, jj, kk));
00688
00689         // *****
00690         // *** > uPSE;
00691         // *****
00692
00693         VAT3(uPSE, ii, jj, kk) =
00694         (
00695             VAT3( uC, ip1, jml, k) * VAT3(oPSE, ii, jj, kk)
00696         + VAT3( oE, i, jml, kpl) * VAT3( uPS, ii, jj, kk)
00697         + VAT3( oN, ip1, jml, kpl) * VAT3( uPE, ii, jj, kk)
00698         ) / VAT3( oC, ip1, jml, kpl);
00699
00700         //fprintf(data, "%19.12E\n", VAT3(uPSE, ii, jj, kk));
00701
00702         // *****
00703         // *** > uPSW;
00704         // *****
00705
00706         VAT3(uPSW, ii, jj, kk) =
00707         (
00708             VAT3( uC, iml, jml, k) * VAT3(oPSW, ii, jj, kk)
00709         + VAT3( oE, iml, jml, kpl) * VAT3( uPS, ii, jj, kk)
00710         + VAT3( oN, iml, jml, kpl) * VAT3( uPW, ii, jj, kk)
00711         ) / VAT3( oC, iml, jml, kpl);
00712
00713         //fprintf(data, "%19.12E\n", VAT3(uPSW, ii, jj, kk));
00714
00715     }
00716 }
00717 }
00718 }
00719
00720
00721
00722 VPUBLIC void VbuildP_op27(int *nxf, int *nyf, int *nzf,
00723     int *nxc, int *nyc, int *nzc,
00724     int *ipc, double *rpc,
00725     double *ac, double *pc) {
00726
00727     MAT2(ac, *nxf * *nyf * *nzf, 1);
00728     MAT2(pc, *nxc * *nyc * *nzc, 1);
00729
00730     WARN_UNTESTED;
00731
00732     VbuildPb_op27(nxf, nyf, nzf,

```

```

00733         nxc, nyc, nzc,
00734         ipc, rpc,
00735
00736         RAT2(ac, 1, 1), RAT2(ac, 1, 2), RAT2(ac, 1, 3),
00737         RAT2(ac, 1, 4),
00738         RAT2(ac, 1, 5), RAT2(ac, 1, 6),
00739         RAT2(ac, 1, 7), RAT2(ac, 1, 8), RAT2(ac, 1, 9), RAT2(ac, 1, 10),
00740         RAT2(ac, 1, 11), RAT2(ac, 1, 12), RAT2(ac, 1, 13), RAT2(ac, 1, 14),
00741         RAT2(pc, 1, 1), RAT2(pc, 1, 2), RAT2(pc, 1, 3), RAT2(pc, 1, 4), RAT2(pc, 1, 5),
00742         RAT2(pc, 1, 6), RAT2(pc, 1, 7), RAT2(pc, 1, 8), RAT2(pc, 1, 9),
00743         RAT2(pc, 1, 10), RAT2(pc, 1, 11), RAT2(pc, 1, 12), RAT2(pc, 1, 13), RAT2(pc, 1, 14),
00744         RAT2(pc, 1, 15), RAT2(pc, 1, 16), RAT2(pc, 1, 17), RAT2(pc, 1, 18),
00745         RAT2(pc, 1, 19), RAT2(pc, 1, 20), RAT2(pc, 1, 21), RAT2(pc, 1, 22), RAT2(pc, 1, 23),
00746         RAT2(pc, 1, 24), RAT2(pc, 1, 25), RAT2(pc, 1, 26), RAT2(pc, 1, 27));
00747     }
00748
00749     VPUBLIC void VbuildPb_op27(int *nxf, int *nyf, int *nzf,
00750         int *nxc, int *nyc, int *nzc,
00751         int *ipc, double *rpc,
00752         double *oC, double *oE, double *oN,
00753         double *uC,
00754         double *oNE, double *oNW,
00755         double *uE, double *uW, double *uN, double *uS,
00756         double *uNE, double *uNW, double *uSE, double *uSW,
00757         double *oPC, double *oPN, double *oPS, double *oPE, double *oPW,
00758         double *oPNE, double *oPNW, double *oPSE, double *oPSW,
00759         double *uPC, double *uPN, double *uPS, double *uPE, double *uPW,
00760         double *uPNE, double *uPNW, double *uPSE, double *uPSW,
00761         double *dPC, double *dPN, double *dPS, double *dPE, double *dPW,
00762         double *dPNE, double *dPNW, double *dPSE, double *dPSW) {
00763
00764         int i, j, k;
00765         int ii, jj, kk;
00766         int im1, ip1;
00767         int im2, ip2;
00768         int jm1, jp1;
00769         int jm2, jp2;
00770         int km1, kp1;
00771         int km2, kp2;
00772         int iim1, iip1;
00773         int jjm1, jjp1;
00774         int kkm1, kkp1;
00775
00776         double won, half, quarter, eighth;
00777
00778         MAT3( oC, *nxf, *nyf, *nzf);
00779         MAT3( oE, *nxf, *nyf, *nzf);
00780         MAT3( oN, *nxf, *nyf, *nzf);
00781         MAT3( uC, *nxf, *nyf, *nzf);
00782         MAT3( oNE, *nxf, *nyf, *nzf);
00783         MAT3( oNW, *nxf, *nyf, *nzf);
00784         MAT3( uE, *nxf, *nyf, *nzf);
00785         MAT3( uW, *nxf, *nyf, *nzf);
00786         MAT3( uN, *nxf, *nyf, *nzf);
00787         MAT3( uS, *nxf, *nyf, *nzf);
00788         MAT3( uNE, *nxf, *nyf, *nzf);
00789         MAT3( uNW, *nxf, *nyf, *nzf);
00790         MAT3( uSE, *nxf, *nyf, *nzf);
00791         MAT3( uSW, *nxf, *nyf, *nzf);
00792         MAT3( oPC, *nxc, *nyc, *nzc);
00793         MAT3( oPN, *nxc, *nyc, *nzc);
00794         MAT3( oPS, *nxc, *nyc, *nzc);
00795         MAT3( oPE, *nxc, *nyc, *nzc);
00796         MAT3( oPW, *nxc, *nyc, *nzc);
00797         MAT3( oPNE, *nxc, *nyc, *nzc);
00798         MAT3( oPNW, *nxc, *nyc, *nzc);
00799         MAT3( oPSE, *nxc, *nyc, *nzc);
00800         MAT3( oPSW, *nxc, *nyc, *nzc);
00801         MAT3( uPC, *nxc, *nyc, *nzc);
00802         MAT3( uPN, *nxc, *nyc, *nzc);
00803         MAT3( uPS, *nxc, *nyc, *nzc);
00804         MAT3( uPE, *nxc, *nyc, *nzc);
00805         MAT3( uPW, *nxc, *nyc, *nzc);
00806         MAT3( uPNE, *nxc, *nyc, *nzc);
00807         MAT3( uPNW, *nxc, *nyc, *nzc);
00808         MAT3( uPSE, *nxc, *nyc, *nzc);
00809         MAT3( uPSW, *nxc, *nyc, *nzc);
00810         MAT3( dPC, *nxc, *nyc, *nzc);
00811         MAT3( dPN, *nxc, *nyc, *nzc);
00812         MAT3( dPS, *nxc, *nyc, *nzc);
00813         MAT3( dPE, *nxc, *nyc, *nzc);

```



```

00814     MAT3( dPW, *nxc, *nyc, *nzc);
00815     MAT3( dPNE, *nxc, *nyc, *nzc);
00816     MAT3( dPNW, *nxc, *nyc, *nzc);
00817     MAT3( dPSE, *nxc, *nyc, *nzc);
00818     MAT3( dPSW, *nxc, *nyc, *nzc);
00819
00820     WARN_UNTESTED;
00821
00822     // Interpolation Stencil
00823     won      = 1.0;
00824     half     = 1.0 / 2.0;
00825     quarter  = 1.0 / 4.0;
00826     eighth   = 1.0 / 8.0;
00827
00828     //fprintf(data, "%s\n", PRINT_FUNC);
00829
00830     for (kk = 2; kk <= *nzc - 1; kk++) {
00831         k = 2 * kk - 1;
00832
00833         for (jj = 2; jj <= *nyc - 1; jj++) {
00834             j = 2 * jj - 1;
00835
00836             for (ii = 2; ii <= *nxc - 1; ii++) {
00837                 i = 2 * ii - 1;
00838
00839                 // Index Computations
00840                 im1 = i - 1;
00841                 ip1 = i + 1;
00842                 im2 = i - 2;
00843                 ip2 = i + 2;
00844                 jm1 = j - 1;
00845                 jp1 = j + 1;
00846                 jm2 = j - 2;
00847                 jp2 = j + 2;
00848                 km1 = k - 1;
00849                 kp1 = k + 1;
00850                 km2 = k - 2;
00851                 kp2 = k + 2;
00852                 iim1 = ii - 1;
00853                 iip1 = ii + 1;
00854                 jjm1 = jj - 1;
00855                 jjp1 = jj + 1;
00856                 kkm1 = kk - 1;
00857                 kkp1 = kk + 1;
00858
00859                 /* *****
00860                 /* *** > oPC;
00861                 /* *****
00862
00863                 VAT3( oPC, ii, jj, kk) = won;
00864
00865                 //fprintf(data, "%19.12E\n", VAT3(oPC, ii, jj, kk));
00866
00867                 /* *****
00868                 /* *** > oPN;
00869                 /* *****
00870
00871                 VAT3( oPN, ii, jj, kk) =
00872                 (
00873                     VAT3( uNE, im1, j, km1)
00874                     + VAT3( uN, i, j, km1)
00875                     + VAT3( uNW, ip1, j, km1)
00876                     + VAT3( oNE, im1, j, k)
00877                     + VAT3( oN, i, j, k)
00878                     + VAT3( oNW, ip1, j, k)
00879                     + VAT3( uSW, i, jp1, k)
00880                     + VAT3( uS, i, jp1, k)
00881                     + VAT3( uSE, i, jp1, k)
00882                 ) / (
00883                     VAT3( oC, i, jp1, k)
00884                     - VAT3( oE, im1, jp1, k)
00885                     - VAT3( oE, i, jp1, k)
00886                     - VAT3( uC, i, jp1, km1)
00887                     - VAT3( uE, im1, jp1, km1)
00888                     - VAT3( uW, ip1, jp1, km1)
00889                     - VAT3( uC, i, jp1, k)
00890                     - VAT3( uW, i, jp1, k)
00891                     - VAT3( uE, i, jp1, k)
00892                 );
00893
00894                 //fprintf(data, "%19.12E\n", VAT3(oPN, ii, jj, kk));

```

```

00895
00896
00897     /* *****
00898     /* *** > oPS;
00899     /* *****
00900
00901     VAT3( oPS,  ii,  jj,  kk) =
00902     (
00903         VAT3( uSE, im1,  j, km1)
00904         + VAT3( uS,  i,  j, km1)
00905         + VAT3( uSW, ip1,  j, km1)
00906         + VAT3( oNW, i, jml,  k)
00907         + VAT3( oN,  i, jml,  k)
00908         + VAT3( oNE, i, jml,  k)
00909         + VAT3( uNW, i, jml,  k)
00910         + VAT3( uN,  i, jml,  k)
00911         + VAT3( uNE, i, jml,  k)
00912     ) / (
00913         VAT3( oC,  i, jml,  k)
00914         - VAT3( oE, im1, jml,  k)
00915         - VAT3( oE,  i, jml,  k)
00916         - VAT3( uC,  i, jml, km1)
00917         - VAT3( uE, im1, jml, km1)
00918         - VAT3( uW, ip1, jml, km1)
00919         - VAT3( uC,  i, jml,  k)
00920         - VAT3( uW,  i, jml,  k)
00921         - VAT3( uE,  i, jml,  k)
00922     );
00923
00924     //fprintf(data, "%19.12E\n", VAT3(oPS, ii, jj, kk));
00925
00926     /* *****
00927     /* *** > oPE;
00928     /* *****
00929
00930     VAT3( oPE,  ii,  jj,  kk) =
00931     (
00932         VAT3( uSE,  i, jpl, km1)
00933         + VAT3( oNW, ip1,  j,  k)
00934         + VAT3( uNW, ip1,  j,  k)
00935         + VAT3( uE,  i,  j, km1)
00936         + VAT3( oE,  i,  j,  k)
00937         + VAT3( uW, ip1,  j,  k)
00938         + VAT3( uNE, i, jml, km1)
00939         + VAT3( oNE, i, jml,  k)
00940         + VAT3( uSW, ip1,  j,  k)
00941     ) / (
00942         VAT3( oC, ip1,  j,  k)
00943         - VAT3( uC, ip1,  j, km1)
00944         - VAT3( uC, ip1,  j,  k)
00945         - VAT3( oN, ip1,  j,  k)
00946         - VAT3( uS, ip1, jpl, km1)
00947         - VAT3( uN, ip1,  j,  k)
00948         - VAT3( oN, ip1, jml,  k)
00949         - VAT3( uN, ip1, jml, km1)
00950         - VAT3( uS, ip1,  j,  k)
00951     );
00952
00953     //fprintf(data, "%19.12E\n", VAT3(oPE, ii, jj, kk));
00954
00955     /* *****
00956     /* *** > oPW;
00957     /* *****
00958
00959     VAT3( oPW,  ii,  jj,  kk) =
00960     (
00961         VAT3( uSW,  i, jpl, km1)
00962         + VAT3( oNE, im1,  j,  k)
00963         + VAT3( uNE, im1,  j,  k)
00964         + VAT3( uW,  i,  j, km1)
00965         + VAT3( oE, im1,  j,  k)
00966         + VAT3( uE, im1,  j,  k)
00967         + VAT3( uNW, i, jml, km1)
00968         + VAT3( oNW, i, jml,  k)
00969         + VAT3( uSE, im1,  j,  k)
00970     ) / (
00971         VAT3( oC, im1,  j,  k)
00972         - VAT3( uC, im1,  j, km1)
00973         - VAT3( uC, im1,  j,  k)
00974         - VAT3( oN, im1,  j,  k)
00975         - VAT3( uS, im1, jpl, km1)
00976         - VAT3( uN, im1,  j,  k)

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```

00976         - VAT3( oN, im1, jml, k)
00977         - VAT3( uN, im1, jml, kml)
00978         - VAT3( uS, im1, j, k)
00979     );
00980
00981     //fprintf(data, "%19.12E\n", VAT3(oPW, ii, jj, kk));
00982
00983     /* *****
00984     /* *** > oPNE;
00985     /* *****
00986
00987     VAT3(oPNE, ii, jj, kk) =
00988     (
00989         VAT3( uNE, i, j, kml)
00990         + VAT3( oNE, i, j, k)
00991         + VAT3( uSW, ip1, jpl, k)
00992         + (
00993             VAT3( uN, ip1, j, kml)
00994             + VAT3( oN, ip1, j, k)
00995             + VAT3( uS, ip1, jpl, k)
00996         )
00997         * VAT3( oPE, ii, jj, kk)
00998         + (
00999             VAT3( uE, i, jpl, kml)
01000             + VAT3( oE, i, jpl, k)
01001             + VAT3( uW, ip1, jpl, k)
01002         )
01003         * VAT3( oPN, ii, jj, kk)
01004     ) / (
01005         VAT3( oC, ip1, jpl, k)
01006         - VAT3( uC, ip1, jpl, kml)
01007         - VAT3( uC, ip1, jpl, k)
01008     );
01009
01010     //fprintf(data, "%19.12E\n", VAT3(oPNE, ii, jj, kk));
01011
01012     /* *****
01013     /* *** > oPNW;
01014     /* *****
01015
01016     VAT3(oPNW, ii, jj, kk) =
01017     (
01018         VAT3( uNW, i, j, kml)
01019         + VAT3( oNW, i, j, k)
01020         + VAT3( uSE, im1, jpl, k)
01021         + (
01022             VAT3( uN, im1, j, kml)
01023             + VAT3( oN, im1, j, k)
01024             + VAT3( uS, im1, jpl, k)
01025         )
01026         * VAT3( oPW, ii, jj, kk)
01027         + (
01028             VAT3( uW, i, jpl, kml)
01029             + VAT3( oE, im1, jpl, k)
01030             + VAT3( uE, im1, jpl, k)
01031         )
01032         * VAT3( oPN, ii, jj, kk)
01033     ) / (
01034         VAT3( oC, im1, jpl, k)
01035         - VAT3( uC, im1, jpl, kml)
01036         - VAT3( uC, im1, jpl, k)
01037     );
01038
01039     //fprintf(data, "%19.12E\n", VAT3(oPNW, ii, jj, kk));
01040
01041     /* *****
01042     /* *** > oPSE;
01043     /* *****
01044
01045     VAT3(oPSE, ii, jj, kk) =
01046     (
01047         VAT3( uSE, i, j, kml)
01048         + VAT3( oNW, ip1, jml, k)
01049         + VAT3( uNW, ip1, jml, k)
01050         + (
01051             VAT3( uS, ip1, j, kml)
01052             + VAT3( oN, ip1, jml, k)
01053             + VAT3( uN, ip1, jml, k)
01054         )
01055         * VAT3( oPE, ii, jj, kk)
01056         + (

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```

01057             VAT3( uE, i, jml, kml)
01058             + VAT3( oE, i, jml, k)
01059             + VAT3( uW, ip1, jml, k)
01060         )
01061         * VAT3( oPS, ii, jj, kk)
01062     ) / (
01063         VAT3( oC, ip1, jml, k)
01064         - VAT3( uC, ip1, jml, kml)
01065         - VAT3( uC, ip1, jml, k)
01066     );
01067
01068     //fprintf(data, "%19.12E\n", VAT3(oPSE, ii, jj, kk));
01069
01070     /* *****
01071     /* *** > oPSW;
01072     /* *****
01073
01074     VAT3(oPSW, ii, jj, kk) =
01075     (
01076         VAT3( uSW, i, j, kml)
01077         + VAT3( oNE, im1, jml, k)
01078         + VAT3( uNE, im1, jml, k)
01079         + (
01080             VAT3( uS, im1, j, kml)
01081             + VAT3( oN, im1, jml, k)
01082             + VAT3( uN, im1, jml, k)
01083         )
01084         * VAT3( oPW, ii, jj, kk)
01085         + (
01086             VAT3( uW, i, jml, kml)
01087             + VAT3( oE, im1, jml, k)
01088             + VAT3( uE, im1, jml, k)
01089         )
01090         * VAT3( oPS, ii, jj, kk)
01091     ) / (
01092         VAT3( oC, im1, jml, k)
01093         - VAT3( uC, im1, jml, kml)
01094         - VAT3( uC, im1, jml, k)
01095     );
01096
01097     //fprintf(data, "%19.12E\n", VAT3(oPSW, ii, jj, kk));
01098
01099     /* *****
01100     /* *** > dPC;
01101     /* *****
01102
01103     VAT3( dPC, ii, jj, kk) =
01104     (
01105         VAT3( uNW, i, j, kml)
01106         + VAT3( uW, i, j, kml)
01107         + VAT3( uSW, i, j, kml)
01108         + VAT3( uN, i, j, kml)
01109         + VAT3( uC, i, j, kml)
01110         + VAT3( uS, i, j, kml)
01111         + VAT3( uNE, i, j, kml)
01112         + VAT3( uE, i, j, kml)
01113         + VAT3( uSE, i, j, kml)
01114     ) / (
01115         VAT3( oC, i, j, kml)
01116         - VAT3( oN, i, j, kml)
01117         - VAT3( oN, i, jml, kml)
01118         - VAT3( oNW, i, j, kml)
01119         - VAT3( oE, im1, j, kml)
01120         - VAT3( oNE, im1, jml, kml)
01121         - VAT3( oNE, i, j, kml)
01122         - VAT3( oE, i, j, kml)
01123         - VAT3( oNW, ip1, jml, kml)
01124     );
01125
01126     //fprintf(data, "%19.12E\n", VAT3(dPC, ii, jj, kk));
01127
01128     /* *****
01129     /* *** > dPN;
01130     /* *****
01131
01132     VAT3( dPN, ii, jj, kk) =
01133     (
01134         VAT3( uSW, i, jpl, kml)
01135         + VAT3( uS, i, jpl, kml)
01136         + VAT3( uSE, i, jpl, kml)
01137         + (

```

```

01138         VAT3( oNE, im1, j, km1)
01139         + VAT3( oN, i, j, km1)
01140         + VAT3( oNW, ip1, j, km1)
01141     )
01142     * VAT3( dPC, ii, jj, kk)
01143     + (
01144         VAT3( uW, i, jpl, km1)
01145         + VAT3( uC, i, jpl, km1)
01146         + VAT3( uE, i, jpl, km1)
01147     )
01148     * VAT3( oPN, ii, jj, kk)
01149 ) / (
01150     VAT3( oC, i, jpl, km1)
01151     - VAT3( oE, im1, jpl, km1)
01152     - VAT3( oE, i, jpl, km1)
01153 );
01154
01155 //fprintf(data, "%19.12E\n", VAT3(dPN, ii, jj, kk));
01156
01157 /* *****
01158 /* *** > dPS;
01159 /* *****
01160
01161 VAT3( dPS, ii, jj, kk) =
01162 (
01163     VAT3( uNW, i, jml, km1)
01164     + VAT3( uN, i, jml, km1)
01165     + VAT3( uNE, i, jml, km1)
01166     + (
01167         VAT3( oNW, i, jml, km1)
01168         + VAT3( oN, i, jml, km1)
01169         + VAT3( oNE, i, jml, km1)
01170     )
01171     * VAT3( dPC, ii, jj, kk)
01172     + (
01173         VAT3( uW, i, jml, km1)
01174         + VAT3( uC, i, jml, km1)
01175         + VAT3( uE, i, jml, km1)
01176     )
01177     * VAT3( oPS, ii, jj, kk)
01178 ) / (
01179     VAT3( oC, i, jml, km1)
01180     - VAT3( oE, im1, jml, km1)
01181     - VAT3( oE, i, jml, km1)
01182 );
01183
01184 //fprintf(data, "%19.12E\n", VAT3(dPS, ii, jj, kk));
01185
01186 /* *****
01187 /* *** > dPE;
01188 /* *****
01189
01190 VAT3( dPE, ii, jj, kk) =
01191 (
01192     VAT3( uNW, ip1, j, km1)
01193     + VAT3( uW, ip1, j, km1)
01194     + VAT3( uSW, ip1, j, km1)
01195     + (
01196         VAT3( uN, ip1, j, km1)
01197         + VAT3( uC, ip1, j, km1)
01198         + VAT3( uS, ip1, j, km1)
01199     )
01200     * VAT3( oPE, ii, jj, kk)
01201     + (
01202         VAT3( oNW, ip1, j, km1)
01203         + VAT3( oE, i, j, km1)
01204         + VAT3( oNE, i, jml, km1)
01205     )
01206     * VAT3( dPC, ii, jj, kk)
01207 ) / (
01208     VAT3( oC, ip1, j, km1)
01209     - VAT3( oN, ip1, j, km1)
01210     - VAT3( oN, ip1, jml, km1)
01211 );
01212
01213 //fprintf(data, "%19.12E\n", VAT3(dPE, ii, jj, kk));
01214
01215 /* *****
01216 /* *** > dPW;
01217 /* *****
01218

```

```

01219     VAT3( dPW, ii, jj, kk) =
01220     (
01221         VAT3( uNE, im1, j, km1)
01222     +   VAT3( uE, im1, j, km1)
01223     +   VAT3( uSE, im1, j, km1)
01224     +   (
01225         VAT3( uN, im1, j, km1)
01226     +   VAT3( uC, im1, j, km1)
01227     +   VAT3( uS, im1, j, km1)
01228     )
01229     * VAT3( oPW, ii, jj, kk)
01230     +   (
01231         VAT3( oNE, im1, j, km1)
01232     +   VAT3( oE, im1, j, km1)
01233     +   VAT3( oNW, i, jml, km1)
01234     )
01235     * VAT3( dPC, ii, jj, kk)
01236     ) / (
01237         VAT3( oC, im1, j, km1)
01238     -   VAT3( oN, im1, j, km1)
01239     -   VAT3( oN, im1, jml, km1)
01240     );
01241
01242     //fprintf(data, "%19.12E\n", VAT3(dPW, ii, jj, kk));
01243
01244     /* *****
01245     /* *** > dPNE;
01246     /* *****
01247
01248     VAT3(dPNE, ii, jj, kk) =
01249     (
01250         VAT3( uSW, ip1, jpl, km1)
01251     +   VAT3( uW, ip1, jpl, km1)
01252     *   VAT3( oPN, ii, jj, kk)
01253     +   VAT3( uS, ip1, jpl, km1)
01254     *   VAT3( oPE, ii, jj, kk)
01255     +   VAT3( uC, ip1, jpl, km1)
01256     *   VAT3( oPNE, ii, jj, kk)
01257     +   VAT3( oNE, i, j, km1)
01258     *   VAT3( dPC, ii, jj, kk)
01259     +   VAT3( oE, i, jpl, km1)
01260     *   VAT3( dPN, ii, jj, kk)
01261     +   VAT3( oN, ip1, j, km1)
01262     *   VAT3( dPE, ii, jj, kk)
01263     )
01264     / VAT3( oC, ip1, jpl, km1);
01265
01266     //fprintf(data, "%19.12E\n", VAT3(dPNE, ii, jj, kk));
01267
01268     /* *****
01269     /* *** > dPNW;
01270     /* *****
01271
01272     VAT3(dPNW, ii, jj, kk) =
01273     (
01274         VAT3( uSE, im1, jpl, km1)
01275     +   VAT3( uE, im1, jpl, km1)
01276     *   VAT3( oPN, ii, jj, kk)
01277     +   VAT3( uS, im1, jpl, km1)
01278     *   VAT3( oPW, ii, jj, kk)
01279     +   VAT3( uC, im1, jpl, km1)
01280     *   VAT3( oPNW, ii, jj, kk)
01281     +   VAT3( oNW, i, j, km1)
01282     *   VAT3( dPC, ii, jj, kk)
01283     +   VAT3( oE, im1, jpl, km1)
01284     *   VAT3( dPN, ii, jj, kk)
01285     +   VAT3( oN, im1, j, km1)
01286     *   VAT3( dPW, ii, jj, kk)
01287     )
01288     / VAT3( oC, im1, jpl, km1);
01289
01290     //fprintf(data, "%19.12E\n", VAT3(dPNW, ii, jj, kk));
01291
01292     /* *****
01293     /* *** > dPSE;
01294     /* *****
01295
01296     VAT3(dPSE, ii, jj, kk) =
01297     (
01298         VAT3( uNW, ip1, jml, km1)
01299     +   VAT3( uW, ip1, jml, km1)

```

```

01300             * VAT3( oPS, ii, jj, kk)
01301             + VAT3( uN, ip1, jml, kml)
01302             * VAT3( oPE, ii, jj, kk)
01303             + VAT3( uC, ip1, jml, kml)
01304             * VAT3( oPSE, ii, jj, kk)
01305             + VAT3( oNW, ip1, jml, kml)
01306             * VAT3( dPC, ii, jj, kk)
01307             + VAT3( oE, i, jml, kml)
01308             * VAT3( dPS, ii, jj, kk)
01309             + VAT3( oN, ip1, jml, kml)
01310             * VAT3( dPE, ii, jj, kk)
01311         )
01312         / VAT3( oC, ip1, jml, kml);
01313
01314         //fprintf(data, "%19.12E\n", VAT3(dPSE, ii, jj, kk));
01315
01316         /* *****
01317         /* *** > dPSW;
01318         /* *****
01319
01320         VAT3(dPSW, ii, jj, kk) =
01321         (
01322             VAT3( uNE, im1, jml, kml)
01323             + VAT3( uE, im1, jml, kml)
01324             * VAT3( oPS, ii, jj, kk)
01325             + VAT3( uN, im1, jml, kml)
01326             * VAT3( oPW, ii, jj, kk)
01327             + VAT3( uC, im1, jml, kml)
01328             * VAT3( oPSW, ii, jj, kk)
01329             + VAT3( oNE, im1, jml, kml)
01330             * VAT3( dPC, ii, jj, kk)
01331             + VAT3( oE, im1, jml, kml)
01332             * VAT3( dPS, ii, jj, kk)
01333             + VAT3( oN, im1, jml, kml)
01334             * VAT3( dPW, ii, jj, kk)
01335         )
01336         / VAT3( oC, im1, jml, kml);
01337
01338         //fprintf(data, "%19.12E\n", VAT3(dPSW, ii, jj, kk));
01339
01340         /* *****
01341         /* *** > uPC;
01342         /* *****
01343
01344         VAT3( uPC, ii, jj, kk) =
01345         (
01346             VAT3( uSE, im1, jpl, k)
01347             + VAT3( uE, im1, j, k)
01348             + VAT3( uNE, im1, jml, k)
01349             + VAT3( uS, i, jpl, k)
01350             + VAT3( uC, i, j, k)
01351             + VAT3( uN, i, jml, k)
01352             + VAT3( uSW, ip1, jpl, k)
01353             + VAT3( uW, ip1, j, k)
01354             + VAT3( uNW, ip1, jml, k)
01355         ) / (
01356             VAT3( oC, i, j, kp1)
01357             - VAT3( oN, i, j, kp1)
01358             - VAT3( oN, i, jml, kp1)
01359             - VAT3( oNW, i, j, kp1)
01360             - VAT3( oE, im1, j, kp1)
01361             - VAT3( oNE, im1, jml, kp1)
01362             - VAT3( oNE, i, j, kp1)
01363             - VAT3( oE, i, j, kp1)
01364             - VAT3( oNW, ip1, jml, kp1)
01365         );
01366
01367         //fprintf(data, "%19.12E\n", VAT3(uPC, ii, jj, kk));
01368
01369         /* *****
01370         /* *** > uPN;
01371         /* *****
01372
01373         VAT3( uPN, ii, jj, kk) =
01374         (
01375             VAT3( uNE, im1, j, k)
01376             + VAT3( uN, i, j, k)
01377             + VAT3( uNW, ip1, j, k)
01378             + (
01379                 VAT3( oNE, im1, j, kp1)
01380                 + VAT3( oN, i, j, kp1)

```

```

01381             + VAT3( oNW, ip1, j, kp1)
01382         )
01383         * VAT3( uPC, ii, jj, kk)
01384     + (
01385         VAT3( uE, im1, jpl, k)
01386         + VAT3( uC, i, jpl, k)
01387         + VAT3( uW, ip1, jpl, k)
01388     )
01389     * VAT3( oPN, ii, jj, kk)
01390 ) / (
01391     VAT3( oC, i, jpl, kp1)
01392     - VAT3( oE, im1, jpl, kp1)
01393     - VAT3( oE, i, jpl, kp1)
01394 );
01395
01396 //fprintf(data, "%19.12E\n", VAT3(uPN, ii, jj, kk));
01397
01398 /* *****
01399 /** *** > uPS;
01400 /** *****
01401
01402 VAT3( uPS, ii, jj, kk) =
01403 (
01404     VAT3( uSE, im1, j, k)
01405     + VAT3( uS, i, j, k)
01406     + VAT3( uSW, ip1, j, k)
01407     + (
01408         VAT3( oNW, i, jml, kp1)
01409     + VAT3( oN, i, jml, kp1)
01410     + VAT3( oNE, i, jml, kp1)
01411     )
01412     * VAT3( uPC, ii, jj, kk)
01413     + (
01414         VAT3( uE, im1, jml, k)
01415     + VAT3( uC, i, jml, k)
01416     + VAT3( uW, ip1, jml, k)
01417     )
01418     * VAT3( oPS, ii, jj, kk)
01419 ) / (
01420     VAT3( oC, i, jml, kp1)
01421     - VAT3( oE, im1, jml, kp1)
01422     - VAT3( oE, i, jml, kp1)
01423 );
01424
01425 //fprintf(data, "%19.12E\n", VAT3(uPS, ii, jj, kk));
01426
01427 /* *****
01428 /** *** > uPE;
01429 /** *****
01430
01431 VAT3( uPE, ii, jj, kk) =
01432 (
01433     VAT3( uSE, i, jpl, k)
01434     + VAT3( uS, ip1, jpl, k)
01435     + VAT3( uNE, i, jml, k)
01436     + (
01437         VAT3( uS, ip1, jpl, k)
01438     + VAT3( uC, ip1, j, k)
01439     + VAT3( uN, ip1, jml, k)
01440     )
01441     * VAT3( oPE, ii, jj, kk)
01442     + (
01443         VAT3( oNW, ip1, j, kp1)
01444     + VAT3( oE, i, j, kp1)
01445     + VAT3( oNE, i, jml, kp1)
01446     )
01447     * VAT3( uPC, ii, jj, kk)
01448 ) / (
01449     VAT3( oC, ip1, j, kp1)
01450     - VAT3( oN, ip1, j, kp1)
01451     - VAT3( oN, ip1, jml, kp1)
01452 );
01453
01454 //fprintf(data, "%19.12E\n", VAT3(uPE, ii, jj, kk));
01455
01456 /* *****
01457 /** *** > uPW;
01458 /** *****
01459
01460 VAT3( uPW, ii, jj, kk) =
01461 (

```



```

01462         VAT3( uSW, i, jpl, k)
01463 + VAT3( uW, i, j, k)
01464 + VAT3( uNW, i, jml, k)
01465 + (
01466     VAT3( uS, iml, jpl, k)
01467 + VAT3( uC, iml, j, k)
01468 + VAT3( uN, iml, jml, k)
01469 )
01470 * VAT3( oPW, ii, jj, kk)
01471 + (
01472     VAT3( oNE, iml, j, kpl)
01473 + VAT3( oE, iml, j, kpl)
01474 + VAT3( oNW, i, jml, kpl)
01475 )
01476 * VAT3( uPC, ii, jj, kk)
01477 ) / (
01478     VAT3( oC, iml, j, kpl)
01479 - VAT3( oN, iml, j, kpl)
01480 - VAT3( oN, iml, jml, kpl)
01481 );
01482
01483 //fprintf(data, "%19.12E\n", VAT3(uPW, ii, jj, kk));
01484
01485 /* *****
01486 /* *** > uPNE;
01487 /* *****
01488
01489 VAT3(uPNE, ii, jj, kk) =
01490 (
01491     VAT3( uNE, i, j, k)
01492 + VAT3( uE, i, jpl, k)
01493 * VAT3( oPN, ii, jj, kk)
01494 + VAT3( uN, ip1, j, k)
01495 * VAT3( oPE, ii, jj, kk)
01496 + VAT3( uC, ip1, jpl, k)
01497 * VAT3( oPNE, ii, jj, kk)
01498 + VAT3( oNE, i, j, kpl)
01499 * VAT3( uPC, ii, jj, kk)
01500 + VAT3( oE, i, jpl, kpl)
01501 * VAT3( uPN, ii, jj, kk)
01502 + VAT3( oN, ip1, j, kpl)
01503 * VAT3( uPE, ii, jj, kk)
01504 )
01505 / VAT3( oC, ip1, jpl, kpl);
01506
01507 //fprintf(data, "%19.12E\n", VAT3(uPNE, ii, jj, kk));
01508
01509 /* *****
01510 /* *** > uPNW;
01511 /* *****
01512
01513 VAT3(uPNW, ii, jj, kk) =
01514 (
01515     VAT3( uNW, i, j, k)
01516 + VAT3( uW, i, jpl, k)
01517 * VAT3( oPN, ii, jj, kk)
01518 + VAT3( uN, iml, j, k)
01519 * VAT3( oPW, ii, jj, kk)
01520 + VAT3( uC, iml, jpl, k)
01521 * VAT3( oPNW, ii, jj, kk)
01522 + VAT3( oNW, i, j, kpl)
01523 * VAT3( uPC, ii, jj, kk)
01524 + VAT3( oE, iml, jpl, kpl)
01525 * VAT3( uPN, ii, jj, kk)
01526 + VAT3( oN, iml, j, kpl)
01527 * VAT3( uPW, ii, jj, kk)
01528 )
01529 / VAT3( oC, iml, jpl, kpl);
01530
01531 //fprintf(data, "%19.12E\n", VAT3(uPNW, ii, jj, kk));
01532
01533 /* *****
01534 /* *** > uPSE;
01535 /* *****
01536
01537 VAT3(uPSE, ii, jj, kk) =
01538 (
01539     VAT3( uSE, i, j, k)
01540 + VAT3( uE, i, jml, k)
01541 * VAT3( oPS, ii, jj, kk)
01542 + VAT3( uS, ip1, j, k)

```

```

01543         * VAT3( oPE, ii, jj, kk)
01544         + VAT3( uC, ip1, jml, k)
01545         * VAT3(oPSE, ii, jj, kk)
01546         + VAT3( oNW, ip1, jml, kp1)
01547         * VAT3( uPC, ii, jj, kk)
01548         + VAT3( oE, i, jml, kp1)
01549         * VAT3( uPS, ii, jj, kk)
01550         + VAT3( oN, ip1, jml, kp1)
01551         * VAT3( uPE, ii, jj, kk)
01552     )
01553     / VAT3( oC, ip1, jml, kp1);
01554
01555     //fprintf(data, "%19.12E\n", VAT3(uPSE, ii, jj, kk));
01556
01557     /* *****
01558     /* *** > uPSW;
01559     /* *****
01560
01561     VAT3(uPSW, ii, jj, kk) =
01562     (
01563         VAT3( uSW, i, j, k)
01564         + VAT3( uW, i, jml, k)
01565         * VAT3( oPS, ii, jj, kk)
01566         + VAT3( uS, im1, j, k)
01567         * VAT3( oPW, ii, jj, kk)
01568         + VAT3( uC, im1, jml, k)
01569         * VAT3(oPSW, ii, jj, kk)
01570         + VAT3( oNE, im1, jml, kp1)
01571         * VAT3( uPC, ii, jj, kk)
01572         + VAT3( oE, im1, jml, kp1)
01573         * VAT3( uPS, ii, jj, kk)
01574         + VAT3( oN, im1, jml, kp1)
01575         * VAT3( uPW, ii, jj, kk)
01576     )
01577     / VAT3( oC, im1, jml, kp1);
01578
01579     //fprintf(data, "%19.12E\n", VAT3(uPSW, ii, jj, kk));
01580
01581     }
01582 }
01583 }
01584 }

```

9.121 buildPd.h

```

00001
00050 #ifndef _BUILDPD_H_
00051 #define _BUILDPD_H_
00052
00053 #include "apbscfg.h"
00054
00055 #include "malloc/malloc.h"
00056
00057 #include "generic/vhal.h"
00058 #include "generic/vmatrix.h"
00059
00060 VEXTERN void VbuildP(
00061     int    *nxf,
00062     int    *nyf,
00063     int    *nzf,
00064     int    *nxc,
00065     int    *nyc,
00066     int    *nzc,
00067     int    *mgpprol,
00068     int    *ipc,
00069     double *rpc,
00070     double *pc,
00071     double *ac,
00072     double *xf,
00073     double *yf,
00074     double *zf
00075 );
00076
00077 VEXTERN void VbuildP_trilin(
00078     int *nxf,
00079     int *nyf,
00080     int *nzf,
00081     int *nxc,

```

```
00082         int *nyc,
00083         int *nzc,
00084         double *pc,
00085         double *xf,
00086         double *yf,
00087         double *zf
00088     );
00089
00090 VEXTERNC void VbuildPb_trilin(
00091     int     *nxf,
00092     int     *nyf,
00093     int     *nzf,
00094     int     *nxc,
00095     int     *nyc,
00096     int     *nzc,
00097     double *oPC,
00098     double *oPN,
00099     double *oPS,
00100     double *oPE,
00101     double *oPW,
00102     double *oPNE,
00103     double *oPNW,
00104     double *oPSE,
00105     double *oPSW,
00106     double *uPC,
00107     double *uPN,
00108     double *uPS,
00109     double *uPE,
00110     double *uPW,
00111     double *uPNE,
00112     double *uPNW,
00113     double *uPSE,
00114     double *uPSW,
00115     double *dPC,
00116     double *dPN,
00117     double *dPS,
00118     double *dPE,
00119     double *dPW,
00120     double *dPNE,
00121     double *dPNW,
00122     double *dPSE,
00123     double *dPSW,
00124     double *xf,
00125     double *yf,
00126     double *zf
00127 );
00128
00129 VEXTERNC void VbuildP_op7(
00130     int     *nxf,
00131     int     *nyf,
00132     int     *nzf,
00133     int     *nxc,
00134     int     *nyc,
00135     int     *nzc,
00136     int     *ipc,
00137     double *rpc,
00138     double *ac,
00139     double *pc
00140 );
00141
00142 VEXTERNC void VbuildPb_op7(
00143     int     *nxf,
00144     int     *nyf,
00145     int     *nzf,
00146     int     *nxc,
00147     int     *nyc,
00148     int     *nzc,
00149     int     *ipc,
00150     double *rpc,
00151     double *oC,
00152     double *oE,
00153     double *oN,
00154     double *uC,
00155     double *oPC,
00156     double *oPN,
00157     double *oPS,
00158     double *oPE,
00159     double *oPW,
00160     double *oPNE,
00161     double *oPNW,
00162     double *oPSE,
```

```
00163         double *oPSW,
00164         double *uPC,
00165         double *uPN,
00166         double *uPS,
00167         double *uPE,
00168         double *uPW,
00169         double *uPNE,
00170         double *uPNW,
00171         double *uPSE,
00172         double *uPSW,
00173         double *dPC,
00174         double *dPN,
00175         double *dPS,
00176         double *dPE,
00177         double *dPW,
00178         double *dPNE,
00179         double *dPNW,
00180         double *dPSE,
00181         double *dPSW
00182 );
00183
00184 VEXTERNC void VbuildP_op27(
00185         int *nxf,
00186         int *nyf,
00187         int *nzf,
00188         int *nxc,
00189         int *nyc,
00190         int *nzc,
00191         int *ipc,
00192         double *rpc,
00193         double *ac,
00194         double *pc
00195 );
00196
00197 VEXTERNC void VbuildPh_op27(
00198         int *nxf,
00199         int *nyf,
00200         int *nzf,
00201         int *nxc,
00202         int *nyc,
00203         int *nzc,
00204         int *ipc,
00205         double *rpc,
00206         double *oC,
00207         double *oE,
00208         double *oN,
00209         double *uC,
00210         double *oNE,
00211         double *oNW,
00212         double *uE,
00213         double *uW,
00214         double *uN,
00215         double *uS,
00216         double *uNE,
00217         double *uNW,
00218         double *uSE,
00219         double *uSW,
00220         double *oPC,
00221         double *oPN,
00222         double *oPS,
00223         double *oPE,
00224         double *oPW,
00225         double *oPNE,
00226         double *oPNW,
00227         double *oPSE,
00228         double *oPSW,
00229         double *uPC,
00230         double *uPN,
00231         double *uPS,
00232         double *uPE,
00233         double *uPW,
00234         double *uPNE,
00235         double *uPNW,
00236         double *uPSE,
00237         double *uPSW,
00238         double *dPC,
00239         double *dPN,
00240         double *dPS,
00241         double *dPE,
00242         double *dPW,
00243         double *dPNE,
```

```

00244             double *dPNW,
00245             double *dPSE,
00246             double *dPSW
00247 );
00248
00249 #endif /* _BUILDPD_H_ */

```

9.122 cgd.c

```

00001
00055 #include "cgd.h"
00056
00057 VPUBLIC void Vcghs(int *nx, int *ny, int *nz,
00058                  int *ipc, double *rpc,
00059                  double *ac, double *cc, double *fc,
00060                  double *x, double *p, double *ap, double *r,
00061                  int *itmax, int *iters,
00062                  double *errtol, double *omega,
00063                  int *iresid, int *iadjoint) {
00064
00065     double rsnrm, pAp, denom;
00066     double rhok1, rhok2, alpha, beta;
00067
00068     // Setup for the looping
00069     *iters = 0;
00070
00071     if (*iters >= *itmax && *iresid == 0)
00072         return;
00073
00074     Vmresid(nx, ny, nz, ipc, rpc, ac, cc, fc, x, r);
00075     denom = Vxnorm2(nx, ny, nz, r);
00076
00077     if (denom == 0.0)
00078         return;
00079
00080     if (*iters >= *itmax)
00081         return;
00082
00083     while(1) {
00084
00085         // Compute/check the current stopping test
00086         rhok2 = Vxdot(nx, ny, nz, r, r);
00087         rsnrm = VSQRT(rhok2);
00088
00089         if (rsnrm / denom <= *errtol)
00090             break;
00091
00092         if (*iters >= *itmax)
00093             break;
00094
00095         // Form new direction vector from old one and residual
00096         if (*iters == 0) {
00097             Vxcopy(nx, ny, nz, r, p);
00098         } else {
00099             beta = rhok2 / rhok1;
00100             alpha = 1.0 / beta;
00101             Vxaxpy(nx, ny, nz, &alpha, r, p);
00102             Vxscal(nx, ny, nz, &beta, p);
00103         }
00104
00105         // Linear case: alpha which minimizes energy norm of error
00106         Vmatvec(nx, ny, nz, ipc, rpc, ac, cc, p, ap);
00107         pAp = Vxdot(nx, ny, nz, p, ap);
00108         alpha = rhok2 / pAp;
00109
00110         // Save rhok2 for next iteration
00111         rhok1 = rhok2;
00112
00113         // Update solution in direction p of length alpha
00114         Vxaxpy(nx, ny, nz, &alpha, p, x);
00115
00116         // Update residual
00117         alpha = -alpha;
00118         Vxaxpy(nx, ny, nz, &alpha, ap, r);
00119
00120         // some bookkeeping
00121         (*iters)++;
00122     }

```

```
00123 }
```

9.123 cgd.h

```
00001
00050 #ifndef _CGD_H_
00051 #define _CGD_H_
00052
00053 #include "apbscfg.h"
00054
00055 #include "malloc/malloc.h"
00056
00057 #include "generic/vhal.h"
00058 #include "pmgc/matvecd.h"
00059 #include "pmgc/mikpckd.h"
00060
00061 VEXTERNC void Vcghs(
00062     int *nx,
00063     int *ny,
00064     int *nz,
00065     int *ipc,
00066     double *rpc,
00067     double *ac,
00068     double *cc,
00069     double *fc,
00070     double *x,
00071     double *p,
00072     double *ap,
00073     double *r,
00074     int *itmax,
00075     int *iters,
00076     double *errtol,
00077     double *omega,
00078     int *iresid,
00079     int *iadjoint
00080 );
00081
00082 #endif /* _CGD_H_ */
```

9.124 gsd.c

```
00001
00055 #include "gsd.h"
00056
00057 VPUBLIC void Vgsrb(int *nx, int *ny, int *nz,
00058     int *ipc, double *rpc,
00059     double *ac, double *cc, double *fc,
00060     double *x, double *w1, double *w2, double *r,
00061     int *itmax, int *iters,
00062     double *errtol, double *omega,
00063     int *iresid, int *iadjoint) {
00064
00065     int numdia;
00066
00067     MAT2(ac, *nx * *ny * *nz, 1);
00068
00069     // Do in one step ***
00070     numdia = VAT(ipc, 11);
00071     if (numdia == 7) {
00072         Vgsrb7x(nx, ny, nz,
00073             ipc, rpc,
00074             RAT2(ac, 1,1), cc, fc,
00075             RAT2(ac, 1,2), RAT2(ac, 1,3), RAT2(ac, 1,4),
00076             x, w1, w2, r,
00077             itmax, iters, errtol, omega, iresid, iadjoint);
00078     } else if (numdia == 27) {
00079         Vgsrb27x(nx, ny, nz,
00080             ipc, rpc,
00081             RAT2(ac, 1, 1), cc, fc,
00082             RAT2(ac, 1, 2), RAT2(ac, 1, 3), RAT2(ac, 1, 4),
00083             RAT2(ac, 1, 5), RAT2(ac, 1, 6),
00084             RAT2(ac, 1, 7), RAT2(ac, 1, 8), RAT2(ac, 1, 9), RAT2(ac, 1,10),
00085             RAT2(ac, 1,11), RAT2(ac, 1,12), RAT2(ac, 1,13), RAT2(ac, 1,14),
00086             x, w1, w2, r,
00087             itmax, iters, errtol, omega, iresid, iadjoint);
00088     } else {
```

```

00089     Vnm_print(2, "GSRB: invalid stencil type given...\n");
00090 }
00091 }
00092
00093
00094
00095 VPUBLIC void Vgsrb7x(int *nx,int *ny,int *nz,
00096     int *ipc, double *rpc,
00097     double *oC, double *cc, double *fc,
00098     double *oE, double *oN, double *uC,
00099     double *x, double *w1, double *w2, double *r,
00100     int *itmax, int *iters,
00101     double *errtol, double *omega,
00102     int *iresid, int *iadjoint) {
00103
00104     int i, j, k, ioff;
00105
00106     MAT3(cc, *nx, *ny, *nz);
00107     MAT3(fc, *nx, *ny, *nz);
00108     MAT3( x, *nx, *ny, *nz);
00109     MAT3(w1, *nx, *ny, *nz);
00110     MAT3(w2, *nx, *ny, *nz);
00111     MAT3( r, *nx, *ny, *nz);
00112
00113     MAT3(oE, *nx, *ny, *nz);
00114     MAT3(oN, *nx, *ny, *nz);
00115     MAT3(uC, *nx, *ny, *nz);
00116     MAT3(oC, *nx, *ny, *nz);
00117
00118     for (*iters=1; *iters<=*itmax; (*iters)++) {
00119
00120         // Do the red points ***
00121         #pragma omp parallel for private(i, j, k, ioff)
00122         for (k=2; k<=*nz-1; k++) {
00123             for (j=2; j<=*ny-1; j++) {
00124                 ioff = (1 - *iadjoint) * ( (j + k + 2) % 2)
00125                     + ( *iadjoint) * (1 - (j + k + 2) % 2);
00126                 for (i=2+ioff; i<=*nx-1; i+=2) {
00127                     VAT3(x, i, j, k) = (
00128                         VAT3(fc, i, j, k)
00129                         + VAT3(oN, i, j, k) * VAT3(x, i, j+1, k)
00130                         + VAT3(oN, i, j-1, k) * VAT3(x, i, j-1, k)
00131                         + VAT3(oE, i, j, k) * VAT3(x, i+1, j, k)
00132                         + VAT3(oE, i-1, j, k) * VAT3(x, i-1, j, k)
00133                         + VAT3( uC, i, j, k-1) * VAT3(x, i, j, k-1)
00134                         + VAT3( uC, i, j, k) * VAT3(x, i, j, k+1)
00135                         ) / (VAT3(oC, i, j, k) + VAT3(cc, i, j, k));
00136                 }
00137             }
00138         }
00139
00140         // Do the black points
00141         #pragma omp parallel for private(i, j, k, ioff)
00142         for (k=2; k<=*nz-1; k++) {
00143             for (j=2; j<=*ny-1; j++) {
00144                 ioff = ( *iadjoint) * ( (j + k + 2) % 2 )
00145                     + (1 - *iadjoint) * (1 - (j + k + 2) % 2 );
00146                 for (i=2+ioff; i<=*nx-1; i+=2) {
00147                     VAT3(x, i, j, k) = (
00148                         VAT3(fc, i, j, k)
00149                         + VAT3(oN, i, j, k) * VAT3(x, i, j+1, k)
00150                         + VAT3(oN, i, j-1, k) * VAT3(x, i, j-1, k)
00151                         + VAT3(oE, i, j, k) * VAT3(x, i+1, j, k)
00152                         + VAT3(oE, i-1, j, k) * VAT3(x, i-1, j, k)
00153                         + VAT3( uC, i, j, k-1) * VAT3(x, i, j, k-1)
00154                         + VAT3( uC, i, j, k) * VAT3(x, i, j, k+1)
00155                         ) / (VAT3(oC, i, j, k) + VAT3(cc, i, j, k));
00156                 }
00157             }
00158         }
00159     }
00160
00161     if (*iresid == 1)
00162         Vmresid7_ls(nx, ny, nz, ipc, rpc, oC, cc, fc, oE, oN, uC, x, r);
00163 }
00164
00165
00166
00167 VPUBLIC void Vgsrb27x(int *nx,int *ny,int *nz,
00168     int *ipc, double *rpc,
00169     double *oC, double *cc, double *fc,

```

```

00170     double *oE, double *oN, double *uC, double *oNE, double *oNW,
00171     double *uE, double *uW, double *uN, double *uS,
00172     double *uNE, double *uNW, double *uSE, double *uSW,
00173     double *x, double *w1, double *w2, double *r,
00174     int *itmax, int *iters,
00175     double *errtol, double *omega,
00176     int *iresid, int *iadjoint) {
00177
00178     int i, j, k;
00179     int i1, j1, k1;
00180     int i2, j2, k2;
00181     int ioff;
00182     int istep;
00183
00184     double tmpO, tmpU, tmpD;
00185
00186     MAT3( cc, *nx, *ny, *nz);
00187     MAT3( fc, *nx, *ny, *nz);
00188     MAT3( x, *nx, *ny, *nz);
00189     MAT3( w1, *nx, *ny, *nz);
00190     MAT3( w2, *nx, *ny, *nz);
00191     MAT3( r, *nx, *ny, *nz);
00192
00193     MAT3( oE, *nx, *ny, *nz);
00194     MAT3( oN, *nx, *ny, *nz);
00195     MAT3( uC, *nx, *ny, *nz);
00196     MAT3( oC, *nx, *ny, *nz);
00197
00198     MAT3( oNE, *nx, *ny, *nz);
00199     MAT3( oNW, *nx, *ny, *nz);
00200
00201     MAT3( uE, *nx, *ny, *nz);
00202     MAT3( uW, *nx, *ny, *nz);
00203     MAT3( uN, *nx, *ny, *nz);
00204     MAT3( uS, *nx, *ny, *nz);
00205     MAT3( uNE, *nx, *ny, *nz);
00206     MAT3( uNW, *nx, *ny, *nz);
00207     MAT3( uSE, *nx, *ny, *nz);
00208     MAT3( uSW, *nx, *ny, *nz);
00209
00210     // Do the gauss-seidel iteration itmax times
00211
00212     /*
00213     i1 = (1 - *iadjoint) * 2 + ( *iadjoint) * (*nx - 1);
00214     i2 = ( *iadjoint) * 2 + (1 - *iadjoint) * (*nx - 1);
00215     j1 = (1 - *iadjoint) * 2 + ( *iadjoint) * (*ny - 1);
00216     j2 = ( *iadjoint) * 2 + (1 - *iadjoint) * (*ny - 1);
00217     k1 = (1 - *iadjoint) * 2 + ( *iadjoint) * (*nz - 1);
00218     k2 = ( *iadjoint) * 2 + (1 - *iadjoint) * (*nz - 1);
00219     istep = ( *iadjoint) * (-1) + (1 - *iadjoint) * (1);
00220     */
00221
00222     i1 = (1-*iadjoint) * 2 + *iadjoint * (*nx-1);
00223     i2 = *iadjoint * 2 + (1-*iadjoint) * (*nx-1);
00224     j1 = (1-*iadjoint) * 2 + *iadjoint * (*ny-1);
00225     j2 = *iadjoint * 2 + (1-*iadjoint) * (*ny-1);
00226     k1 = (1-*iadjoint) * 2 + *iadjoint * (*nz-1);
00227     k2 = *iadjoint * 2 + (1-*iadjoint) * (*nz-1);
00228     istep = *iadjoint*(-1) + (1-*iadjoint)*(1);
00229
00230     for (*iters=1; *iters<=*itmax; (*iters)++) {
00231
00232         // #pragma omp parallel for private(i, j, k, ioff, tmpO, tmpU, tmpD)
00233         for (k=2; k<=*nz-1; k++) {
00234
00235             for (j=2; j<=*ny-1; j++) {
00236
00237                 ioff = (1 - *iadjoint) * ( (j + k + 2) % 2)
00238                     + ( *iadjoint) * (1 - (j + k + 2) % 2);
00239
00240                 for (i=2+ioff; i<=*nx-1; i+=2) {
00241
00242                     tmpO =
00243                         + VAT3( oN, i, j, k) * VAT3(x, i, j+1, k)
00244                         + VAT3( oN, i, j-1, k) * VAT3(x, i, j-1, k)
00245                         + VAT3( oE, i, j, k) * VAT3(x, i+1, j, k)
00246                         + VAT3( oE, i-1, j, k) * VAT3(x, i-1, j, k)
00247                         + VAT3( oNE, i, j, k) * VAT3(x, i+1, j+1, k)
00248                         + VAT3( oNW, i, j, k) * VAT3(x, i-1, j+1, k)
00249                         + VAT3( oNW, i+1, j-1, k) * VAT3(x, i+1, j-1, k)
00250                         + VAT3( oNE, i-1, j-1, k) * VAT3(x, i-1, j-1, k);

```



```

00251
00252         tmpU =
00253             + VAT3( uC, i, j, k) * VAT3(x, i, j, k+1)
00254             + VAT3( uN, i, j, k) * VAT3(x, i, j+1, k+1)
00255             + VAT3( uS, i, j, k) * VAT3(x, i, j-1, k+1)
00256             + VAT3( uE, i, j, k) * VAT3(x, i+1, j, k+1)
00257             + VAT3( uW, i, j, k) * VAT3(x, i-1, j, k+1)
00258             + VAT3( uNE, i, j, k) * VAT3(x, i+1, j+1, k+1)
00259             + VAT3( uNW, i, j, k) * VAT3(x, i-1, j+1, k+1)
00260             + VAT3( uSE, i, j, k) * VAT3(x, i+1, j-1, k+1)
00261             + VAT3( uSW, i, j, k) * VAT3(x, i-1, j-1, k+1);
00262
00263         tmpD =
00264             + VAT3( uC, i, j, k-1) * VAT3(x, i, j, k-1)
00265             + VAT3( uS, i, j+1, k-1) * VAT3(x, i, j+1, k-1)
00266             + VAT3( uN, i, j-1, k-1) * VAT3(x, i, j-1, k-1)
00267             + VAT3( uW, i+1, j, k-1) * VAT3(x, i+1, j, k-1)
00268             + VAT3( uE, i-1, j, k-1) * VAT3(x, i-1, j, k-1)
00269             + VAT3( uSW, i+1, j+1, k-1) * VAT3(x, i+1, j+1, k-1)
00270             + VAT3( uSE, i-1, j+1, k-1) * VAT3(x, i-1, j+1, k-1)
00271             + VAT3( uNW, i+1, j-1, k-1) * VAT3(x, i+1, j-1, k-1)
00272             + VAT3( uNE, i-1, j-1, k-1) * VAT3(x, i-1, j-1, k-1);
00273
00274         VAT3(x, i, j, k) = (VAT3(fc, i, j, k) + (tmpO + tmpU + tmpD))
00275             / (VAT3(oC, i, j, k) + VAT3(cc, i, j, k));
00276     }
00277 }
00278 }
00279 }
00280
00281 // #pragma omp parallel for private(i, j, k, ioff, tmpO, tmpU, tmpD)
00282 for (k=2; k<=nz-1; k++) {
00283
00284     for (j=2; j<=ny-1; j++) {
00285
00286         ioff = ( *iadjoint) * ( (j + k + 2) % 2)
00287             + (1 - *iadjoint) * (1 - (j + k + 2) % 2);
00288
00289         for (i=2+ioff; i<=nx-1; i+=2) {
00290
00291             tmpO =
00292                 + VAT3( oN, i, j, k) * VAT3(x, i, j+1, k)
00293                 + VAT3( oN, i, j-1, k) * VAT3(x, i, j-1, k)
00294                 + VAT3( oE, i, j, k) * VAT3(x, i+1, j, k)
00295                 + VAT3( oE, i-1, j, k) * VAT3(x, i-1, j, k)
00296                 + VAT3( oNE, i, j, k) * VAT3(x, i+1, j+1, k)
00297                 + VAT3( oNW, i, j, k) * VAT3(x, i-1, j+1, k)
00298                 + VAT3( oNW, i+1, j-1, k) * VAT3(x, i+1, j-1, k)
00299                 + VAT3( oNE, i-1, j-1, k) * VAT3(x, i-1, j-1, k);
00300
00301             tmpU =
00302                 + VAT3( uC, i, j, k) * VAT3(x, i, j, k+1)
00303                 + VAT3( uN, i, j, k) * VAT3(x, i, j+1, k+1)
00304                 + VAT3( uS, i, j, k) * VAT3(x, i, j-1, k+1)
00305                 + VAT3( uE, i, j, k) * VAT3(x, i+1, j, k+1)
00306                 + VAT3( uW, i, j, k) * VAT3(x, i-1, j, k+1)
00307                 + VAT3( uNE, i, j, k) * VAT3(x, i+1, j+1, k+1)
00308                 + VAT3( uNW, i, j, k) * VAT3(x, i-1, j+1, k+1)
00309                 + VAT3( uSE, i, j, k) * VAT3(x, i+1, j-1, k+1)
00310                 + VAT3( uSW, i, j, k) * VAT3(x, i-1, j-1, k+1);
00311
00312             tmpD =
00313                 + VAT3( uC, i, j, k-1) * VAT3(x, i, j, k-1)
00314                 + VAT3( uS, i, j+1, k-1) * VAT3(x, i, j+1, k-1)
00315                 + VAT3( uN, i, j-1, k-1) * VAT3(x, i, j-1, k-1)
00316                 + VAT3( uW, i+1, j, k-1) * VAT3(x, i+1, j, k-1)
00317                 + VAT3( uE, i-1, j, k-1) * VAT3(x, i-1, j, k-1)
00318                 + VAT3( uSW, i+1, j+1, k-1) * VAT3(x, i+1, j+1, k-1)
00319                 + VAT3( uSE, i-1, j+1, k-1) * VAT3(x, i-1, j+1, k-1)
00320                 + VAT3( uNW, i+1, j-1, k-1) * VAT3(x, i+1, j-1, k-1)
00321                 + VAT3( uNE, i-1, j-1, k-1) * VAT3(x, i-1, j-1, k-1);
00322
00323             VAT3(x, i, j, k) = (VAT3(fc, i, j, k) + (tmpO + tmpU + tmpD))
00324                 / (VAT3(oC, i, j, k) + VAT3(cc, i, j, k));
00325         }
00326     }
00327 }
00328 }
00329
00330 // If specified, return the new residual as well
00331 if (*iresid == 1)

```

```

00332         Vmresid27_ls(nx, ny, nz,
00333                     ipc, rpc,
00334                     oC, cc, fc,
00335                     oE, oN, uC,
00336                     oNE, oNW,
00337                     uE, uW, uN, uS,
00338                     uNE, uNW, uSE, uSW,
00339                     x, r);
00340 }

```

9.125 gsd.h

```

00001
00049 #ifndef _GSD_H_
00050 #define _GSD_H_
00051
00052 #include "apbscfg.h"
00053
00054 #include "malloc/malloc.h"
00055
00056 #include "generic/vhal.h"
00057 #include "generic/vmatrix.h"
00058 #include "pmgc/matvecd.h"
00059
00066 VEXTERNC void Vgsrb(
00067     int    *nx,
00068     int    *ny,
00069     int    *nz,
00070     int    *ipc,
00071     double *rpc,
00072     double *ac,
00073     double *cc,
00074     double *fc,
00075     double *x,
00076     double *wl,
00077     double *w2,
00078     double *r,
00079     int    *itmax,
00080     int    *iters,
00081     double *errtol,
00082     double *omega,
00083     int    *iresid,
00084     int    *iadjoint
00085 );
00086
00087 VEXTERNC void Vgsrb7x(
00088     int    *nx,
00089     int    *ny,
00090     int    *nz,
00091     int    *ipc,
00092     double *rpc,
00093     double *oC,
00094     double *cc,
00095     double *fc,
00096     double *oE,
00097     double *oN,
00098     double *uC,
00099     double *x,
00100     double *wl,
00101     double *w2,
00102     double *r,
00103     int    *itmax,
00104     int    *iters,
00105     double *errtol,
00106     double *omega,
00107     int    *iresid,
00108     int    *iadjoint
00109 );
00110
00111 VEXTERNC void Vgsrb27x(
00112     int    *nx,
00113     int    *ny,
00114     int    *nz,
00115     int    *ipc,
00116     double *rpc,
00117     double *oC,
00118     double *cc,
00119     double *fc,

```

```

00120         double *oE,
00121         double *oN,
00122         double *uC,
00123         double *oNE,
00124         double *oNW,
00125         double *uE,
00126         double *uW,
00127         double *uN,
00128         double *uS,
00129         double *uNE,
00130         double *uNW,
00131         double *uSE,
00132         double *uSW,
00133         double *x,
00134         double *w1,
00135         double *w2,
00136         double *r,
00137         int *itmax,
00138         int *iters,
00139         double *errtol,
00140         double *omega,
00141         int *iresid,
00142         int *iadjoint
00143     );
00144
00145
00146 #endif /* _GSD_H_ */

```

9.126 matvecd.c

```

00001
00055 #include "matvecd.h"
00056
00057 VPUBLIC void Vmatvec(int *nx, int *ny, int *nz,
00058     int *ipc, double *rpc,
00059     double *ac, double *cc,
00060     double *x, double *y) {
00061
00062     int numdia;
00063
00064     // Do in one step
00065     numdia = VAT(ipc, 11);
00066
00067     if (numdia == 7) {
00068         Vmatvec7(nx, ny, nz,
00069             ipc, rpc,
00070             ac, cc,
00071             x, y);
00072     } else if (numdia == 27) {
00073         Vmatvec27(nx, ny, nz,
00074             ipc, rpc,
00075             ac, cc,
00076             x, y);
00077     } else {
00078         Vnm_print(2, "MATVEC: invalid stencil type given...");
00079     }
00080 }
00081
00082 VPUBLIC void Vmatvec7(int *nx, int *ny, int *nz,
00083     int *ipc, double *rpc,
00084     double *ac, double *cc,
00085     double *x, double *y) {
00086
00087     MAT2(ac, *nx * *ny * *nz, 1);
00088
00089     Vmatvec7_ls(nx, ny, nz,
00090         ipc, rpc,
00091         RAT2(ac, 1, 1), cc,
00092         RAT2(ac, 1, 2), RAT2(ac, 1, 3), RAT2(ac, 1, 4),
00093         x, y);
00094 }
00095
00096
00097
00098 VEXTERN void Vmatvec7_ls(int *nx, int *ny, int *nz,
00099     int *ipc, double *rpc,
00100     double *oC, double *cc,
00101     double *oE, double *oN, double *uC,

```

```

00102         double *x, double *y) {
00103
00104     int i, j, k;
00105
00106     MAT3(oE, *nx, *ny, *nz);
00107     MAT3(oN, *nx, *ny, *nz);
00108     MAT3(uC, *nx, *ny, *nz);
00109     MAT3(cc, *nx, *ny, *nz);
00110     MAT3(oC, *nx, *ny, *nz);
00111     MAT3(x, *nx, *ny, *nz);
00112     MAT3(y, *nx, *ny, *nz);
00113
00114     // Do it
00115     #pragma omp parallel for private(i, j, k)
00116     for (k=2; k<=*nz-1; k++) {
00117         for (j=2; j<=*ny-1; j++) {
00118             for (i=2; i<=*nx-1; i++) {
00119                 VAT3(y, i, j, k) =
00120                     - VAT3(oN, i, j, k) * VAT3(x, i, j+1, k)
00121                     - VAT3(oN, i, j-1, k) * VAT3(x, i, j-1, k)
00122                     - VAT3(oE, i, j, k) * VAT3(x, i+1, j, k)
00123                     - VAT3(oE, i-1, j, k) * VAT3(x, i-1, j, k)
00124                     - VAT3(uC, i, j, k-1) * VAT3(x, i, j, k-1)
00125                     - VAT3(uC, i, j, k) * VAT3(x, i, j, k+1)
00126                     + (VAT3(oC, i, j, k) + VAT3(cc, i, j, k)) * VAT3(x, i, j, k);
00127             }
00128         }
00129     }
00130 }
00131
00132
00133
00134 VPUBLIC void Vmatvec27(int *nx, int *ny, int *nz,
00135     int *ipc, double *rpc,
00136     double *ac, double *cc,
00137     double *x, double *y) {
00138
00139     MAT2(ac, *nx * *ny * *nz, 1);
00140
00141     Vmatvec27_1s(nx, ny, nz,
00142         ipc, rpc,
00143         RAT2(ac, 1, 1), cc,
00144         RAT2(ac, 1, 2), RAT2(ac, 1, 3), RAT2(ac, 1, 4),
00145         RAT2(ac, 1, 5), RAT2(ac, 1, 6),
00146         RAT2(ac, 1, 7), RAT2(ac, 1, 8), RAT2(ac, 1, 9), RAT2(ac, 1,10),
00147         RAT2(ac, 1,11), RAT2(ac, 1,12), RAT2(ac, 1,13), RAT2(ac, 1,14),
00148         x, y);
00149 }
00150
00151
00152
00153 VPUBLIC void Vmatvec27_1s(int *nx, int *ny, int *nz,
00154     int *ipc, double *rpc,
00155     double *oC, double *cc,
00156     double *oE, double *oN, double *uC,
00157     double *oNE, double *oNW,
00158     double *uE, double *uW, double *uN, double *uS,
00159     double *uNE, double *uNW, double *uSE, double *uSW,
00160     double *x, double *y) {
00161
00162     int i, j, k;
00163
00164     double tmpO, tmpU, tmpD;
00165
00166     MAT3(cc, *nx, *ny, *nz);
00167     MAT3(x, *nx, *ny, *nz);
00168     MAT3(y, *nx, *ny, *nz);
00169
00170     MAT3(oC, *nx, *ny, *nz);
00171     MAT3(oE, *nx, *ny, *nz);
00172     MAT3(oN, *nx, *ny, *nz);
00173     MAT3(oNE, *nx, *ny, *nz);
00174     MAT3(oNW, *nx, *ny, *nz);
00175
00176     MAT3(uC, *nx, *ny, *nz);
00177     MAT3(uE, *nx, *ny, *nz);
00178     MAT3(uW, *nx, *ny, *nz);
00179     MAT3(uN, *nx, *ny, *nz);
00180     MAT3(uS, *nx, *ny, *nz);
00181     MAT3(uNE, *nx, *ny, *nz);
00182     MAT3(uNW, *nx, *ny, *nz);

```

```

00183     MAT3(uSE, *nx, *ny, *nz);
00184     MAT3(uSW, *nx, *ny, *nz);
00185
00186     // Do it
00187     #pragma omp parallel for private(i, j, k, tmpO, tmpU, tmpD)
00188     for (k=2; k<=*nz-1; k++) {
00189         for (j=2; j<=*ny-1; j++) {
00190             for (i=2; i<=*nx-1; i++) {
00191                 tmpO =
00192                 - VAT3( oN, i, j, k) * VAT3(x, i, j+1, k)
00193                 - VAT3( oN, i, j-1, k) * VAT3(x, i, j-1, k)
00194                 - VAT3( oE, i, j, k) * VAT3(x, i+1, j, k)
00195                 - VAT3( oE, i-1, j, k) * VAT3(x, i-1, j, k)
00196                 - VAT3( oNE, i, j, k) * VAT3(x, i+1, j+1, k)
00197                 - VAT3( oNW, i, j, k) * VAT3(x, i-1, j+1, k)
00198                 - VAT3( oNW, i+1, j-1, k) * VAT3(x, i+1, j-1, k)
00199                 - VAT3( oNE, i-1, j-1, k) * VAT3(x, i-1, j-1, k);
00200
00201                 tmpU =
00202                 - VAT3( uC, i, j, k) * VAT3(x, i, j, k+1)
00203                 - VAT3( uN, i, j, k) * VAT3(x, i, j+1, k+1)
00204                 - VAT3( uS, i, j, k) * VAT3(x, i, j-1, k+1)
00205                 - VAT3( uE, i, j, k) * VAT3(x, i+1, j, k+1)
00206                 - VAT3( uW, i, j, k) * VAT3(x, i-1, j, k+1)
00207                 - VAT3( uNE, i, j, k) * VAT3(x, i+1, j+1, k+1)
00208                 - VAT3( uNW, i, j, k) * VAT3(x, i-1, j+1, k+1)
00209                 - VAT3( uSE, i, j, k) * VAT3(x, i+1, j-1, k+1)
00210                 - VAT3( uSW, i, j, k) * VAT3(x, i-1, j-1, k+1);
00211
00212                 tmpD =
00213                 - VAT3( uC, i, j, k-1) * VAT3(x, i, j, k-1)
00214                 - VAT3( uS, i, j+1, k-1) * VAT3(x, i, j+1, k-1)
00215                 - VAT3( uN, i, j-1, k-1) * VAT3(x, i, j-1, k-1)
00216                 - VAT3( uW, i+1, j, k-1) * VAT3(x, i+1, j, k-1)
00217                 - VAT3( uE, i-1, j, k-1) * VAT3(x, i-1, j, k-1)
00218                 - VAT3( uSW, i+1, j+1, k-1) * VAT3(x, i+1, j+1, k-1)
00219                 - VAT3( uSE, i-1, j+1, k-1) * VAT3(x, i-1, j+1, k-1)
00220                 - VAT3( uNW, i+1, j-1, k-1) * VAT3(x, i+1, j-1, k-1)
00221                 - VAT3( uNE, i-1, j-1, k-1) * VAT3(x, i-1, j-1, k-1);
00222
00223                 VAT3(y, i, j, k) = tmpO + tmpU + tmpD
00224                 + (VAT3(oC, i, j, k) + VAT3(cc, i, j, k)) * VAT3(x, i, j, k);
00225             }
00226         }
00227     }
00228 }
00229
00230
00231
00232 VEXTERNC void Vnmatvec(int *nx, int *ny, int *nz,
00233     int *ipc, double *rpc,
00234     double *ac, double *cc, double *x, double *y, double *w1) {
00235
00236     int numdia;
00237
00238     // Do in one step
00239     numdia = VAT(ipc, 11);
00240
00241     if (numdia == 7) {
00242         Vnmatvec7(nx, ny, nz,
00243             ipc, rpc,
00244             ac, cc,
00245             x, y, w1);
00246     } else if (numdia == 27) {
00247         Vnmatvec27(nx, ny, nz,
00248             ipc, rpc,
00249             ac, cc,
00250             x, y, w1);
00251     } else {
00252         Vnm_print(2, "MATVEC: invalid stencil type given...");
00253     }
00254 }
00255
00256
00257
00258 VPUBLIC void Vnmatvec7(int *nx, int *ny, int *nz,
00259     int *ipc, double *rpc,
00260     double *ac, double *cc,
00261     double *x, double *y, double *w1) {
00262
00263     MAT2(ac, *nx * *ny * *nz, 1);

```

```

00264
00265     WARN_UNTESTED;
00266
00267     Vnmatvecd7_ls(nx, ny, nz,
00268         ipc, rpc,
00269         RAT2(ac, 1, 1), cc,
00270         RAT2(ac, 1, 2), RAT2(ac, 1, 3), RAT2(ac, 1, 4),
00271         x, y, w1);
00272 }
00273
00274
00275
00276 VPUBLIC void Vnmatvecd7_ls(int *nx, int *ny, int *nz,
00277     int *ipc, double *rpc,
00278     double *oC, double *cc,
00279     double *oE, double *oN, double *uC,
00280     double *x, double *y, double *w1) {
00281
00282     int i, j, k;
00283     int ipkey;
00284
00285     MAT3(oE, *nx, *ny, *nz);
00286     MAT3(oN, *nx, *ny, *nz);
00287     MAT3(uC, *nx, *ny, *nz);
00288     MAT3(cc, *nx, *ny, *nz);
00289     MAT3(oC, *nx, *ny, *nz);
00290     MAT3(x, *nx, *ny, *nz);
00291     MAT3(y, *nx, *ny, *nz);
00292     MAT3(w1, *nx, *ny, *nz);
00293
00294     WARN_UNTESTED;
00295
00296     // first get vector nonlinear term to avoid subroutine calls
00297     ipkey = VAT(ipc, 10);
00298     Vc_vec(cc, x, w1, nx, ny, nz, &ipkey);
00299
00300     // The operator
00301     #pragma omp parallel for private(i, j, k)
00302     for (k=2; k<=*nz-1; k++)
00303         for (j=2; j<=*ny-1; j++)
00304             for (i=2; i<=*nx-1; i++)
00305                 VAT3(y, i, j, k) =
00306                     - VAT3(oN, i, j, k) * VAT3(x, i, j+1, k)
00307                     - VAT3(oN, i, j-1, k) * VAT3(x, i, j-1, k)
00308                     - VAT3(oE, i, j, k) * VAT3(x, i+1, j, k)
00309                     - VAT3(oE, i-1, j, k) * VAT3(x, i-1, j, k)
00310                     - VAT3(uC, i, j, k-1) * VAT3(x, i, j, k-1)
00311                     - VAT3(uC, i, j, k) * VAT3(x, i, j, k+1)
00312                     + VAT3(oC, i, j, k) * VAT3(x, i, j, k)
00313                     + VAT3(w1, i, j, k);
00314 }
00315
00316
00317 VPUBLIC void Vnmatvecd27(int *nx, int *ny, int *nz,
00318     int *ipc, double *rpc,
00319     double *ac, double *cc,
00320     double *x, double *y, double *w1) {
00321
00322     MAT2(ac, *nx * *ny * *nz, 1);
00323
00324     WARN_UNTESTED;
00325
00326     // Do in one step
00327     Vnmatvecd27_ls(nx, ny, nz,
00328         ipc, rpc,
00329         RAT2(ac, 1, 1), cc,
00330         RAT2(ac, 1, 2), RAT2(ac, 1, 3), RAT2(ac, 1, 4),
00331         RAT2(ac, 1, 5), RAT2(ac, 1, 6),
00332         RAT2(ac, 1, 7), RAT2(ac, 1, 8), RAT2(ac, 1, 9), RAT2(ac, 1, 10),
00333         RAT2(ac, 1, 11), RAT2(ac, 1, 12), RAT2(ac, 1, 13), RAT2(ac, 1, 14),
00334         x, y, w1);
00335 }
00336
00337
00338
00339 VPUBLIC void Vnmatvecd27_ls(int *nx, int *ny, int *nz,
00340     int *ipc, double *rpc,
00341     double *oC, double *cc,
00342     double *oE, double *oN, double *uC,
00343     double *oNE, double *oNW,
00344     double *uE, double *uW, double *uN, double *uS,

```

```

00345     double *uNE, double *uNW, double *uSE, double *uSW,
00346     double *x, double *y, double *w1) {
00347
00348     int i, j, k;
00349     int ipkey;
00350
00351     double tmpO, tmpU, tmpD;
00352
00353     MAT3( oE, *nx, *ny, *nz);
00354     MAT3( oN, *nx, *ny, *nz);
00355     MAT3( uC, *nx, *ny, *nz);
00356     MAT3( oNE, *nx, *ny, *nz);
00357     MAT3( oNW, *nx, *ny, *nz);
00358     MAT3( uE, *nx, *ny, *nz);
00359     MAT3( uW, *nx, *ny, *nz);
00360     MAT3( uN, *nx, *ny, *nz);
00361     MAT3( uS, *nx, *ny, *nz);
00362     MAT3( uNE, *nx, *ny, *nz);
00363     MAT3( uNW, *nx, *ny, *nz);
00364     MAT3( uSE, *nx, *ny, *nz);
00365     MAT3( uSW, *nx, *ny, *nz);
00366     MAT3( cc, *nx, *ny, *nz);
00367     MAT3( oC, *nx, *ny, *nz);
00368     MAT3( x, *nx, *ny, *nz);
00369     MAT3( y, *nx, *ny, *nz);
00370     MAT3( w1, *nx, *ny, *nz);
00371
00372     WARN_UNTESTED;
00373
00374     // First get vector noNlinear term to avoid subroutine calls
00375     ipkey = VAT(ipc, 10);
00376     Vc_vec(cc, x, w1, nx, ny, nz, &ipkey);
00377
00378     // The operator
00379     #pragma omp parallel for private(i, j, k, tmpO, tmpU, tmpD)
00380     for (k=2; k<=*nz-1; k++) {
00381         for (j=2; j<=*ny-1; j++) {
00382             for(i=2; i<=*nx-1; i++) {
00383
00384                 tmpO =
00385                     - VAT3( oN, i, j, k) * VAT3(x, i, j+1, k)
00386                     - VAT3( oN, i, j-1, k) * VAT3(x, i, j-1, k)
00387                     - VAT3( oE, i, j, k) * VAT3(x, i+1, j, k)
00388                     - VAT3( oE, i-1, j, k) * VAT3(x, i-1, j, k)
00389                     - VAT3( oNE, i, j, k) * VAT3(x, i+1, j+1, k)
00390                     - VAT3( oNW, i, j, k) * VAT3(x, i-1, j+1, k)
00391                     - VAT3( oNW, i+1, j-1, k) * VAT3(x, i+1, j-1, k)
00392                     - VAT3( oNE, i-1, j-1, k) * VAT3(x, i-1, j-1, k);
00393
00394                 tmpU =
00395                     - VAT3( uC, i, j, k) * VAT3(x, i, j, k+1)
00396                     - VAT3( uN, i, j, k) * VAT3(x, i, j+1, k+1)
00397                     - VAT3( uS, i, j, k) * VAT3(x, i, j-1, k+1)
00398                     - VAT3( uE, i, j, k) * VAT3(x, i+1, j, k+1)
00399                     - VAT3( uW, i, j, k) * VAT3(x, i-1, j, k+1)
00400                     - VAT3( uNE, i, j, k) * VAT3(x, i+1, j+1, k+1)
00401                     - VAT3( uNW, i, j, k) * VAT3(x, i-1, j+1, k+1)
00402                     - VAT3( uSE, i, j, k) * VAT3(x, i+1, j-1, k+1)
00403                     - VAT3( uSW, i, j, k) * VAT3(x, i-1, j-1, k+1);
00404
00405                 tmpD =
00406                     - VAT3( uC, i, j, k-1) * VAT3(x, i, j, k-1)
00407                     - VAT3( uS, i, j+1, k-1) * VAT3(x, i, j+1, k-1)
00408                     - VAT3( uN, i, j-1, k-1) * VAT3(x, i, j-1, k-1)
00409                     - VAT3( uW, i+1, j, k-1) * VAT3(x, i+1, j, k-1)
00410                     - VAT3( uE, i-1, j, k-1) * VAT3(x, i-1, j, k-1)
00411                     - VAT3( uSW, i+1, j+1, k-1) * VAT3(x, i+1, j+1, k-1)
00412                     - VAT3( uSE, i-1, j+1, k-1) * VAT3(x, i-1, j+1, k-1)
00413                     - VAT3( uNW, i+1, j-1, k-1) * VAT3(x, i+1, j-1, k-1)
00414                     - VAT3( uNE, i-1, j-1, k-1) * VAT3(x, i-1, j-1, k-1);
00415
00416                 VAT3(y, i, j, k) = tmpO + tmpU + tmpD
00417                     + VAT3(oC, i, j, k) * VAT3(x, i, j, k)
00418                     + VAT3(w1, i, j, k);
00419             }
00420         }
00421     }
00422 }
00423
00424
00425

```

```

00426 VPUBLIC void Vmresid(int *nx, int *ny, int *nz,
00427     int *ipc, double *rpc,
00428     double *ac, double *cc, double *fc,
00429     double *x, double *r) {
00430
00431     int numdia;
00432
00433     // Do in one step
00434     numdia = VAT(ipc, 11);
00435     if (numdia == 7) {
00436         Vmresid7(nx, ny, nz, ipc, rpc, ac, cc, fc, x, r);
00437     } else if (numdia == 27) {
00438         Vmresid27(nx, ny, nz, ipc, rpc, ac, cc, fc, x, r);
00439     } else {
00440         Vnm_print(2, "Vmresid: invalid stencil type given...\n");
00441     }
00442 }
00443
00444
00445
00446 VPUBLIC void Vmresid7(int *nx, int *ny, int *nz,
00447     int *ipc, double *rpc,
00448     double *ac, double *cc, double *fc,
00449     double *x, double *r) {
00450
00451     MAT2(ac, *nx * *ny * *nz, 1);
00452
00453     // Do in one step
00454     Vmresid7_ls(nx, ny, nz,
00455         ipc, rpc,
00456         RAT2(ac, 1,1), cc, fc,
00457         RAT2(ac, 1,2), RAT2(ac, 1,3), RAT2(ac, 1,4),
00458         x,r);
00459 }
00460
00461 VPUBLIC void Vmresid7_ls(int *nx, int *ny, int *nz,
00462     int *ipc, double *rpc,
00463     double *oC, double *cc, double *fc,
00464     double *oE, double *oN, double *uC,
00465     double *x, double *r) {
00466
00467     int i, j, k;
00468
00469     MAT3(oE, *nx, *ny, *nz);
00470     MAT3(oN, *nx, *ny, *nz);
00471     MAT3(uC, *nx, *ny, *nz);
00472     MAT3(cc, *nx, *ny, *nz);
00473     MAT3(fc, *nx, *ny, *nz);
00474     MAT3(oC, *nx, *ny, *nz);
00475     MAT3(x, *nx, *ny, *nz);
00476     MAT3(r, *nx, *ny, *nz);
00477
00478     // Do it
00479     #pragma omp parallel for private(i, j, k)
00480     for (k=2; k<=*nz-1; k++) {
00481         for (j=2; j<=*ny-1; j++) {
00482             for (i=2; i<=*nx-1; i++) {
00483                 VAT3(r, i,j,k) = VAT3(fc, i, j, k)
00484                     + VAT3(oN, i, j, k) * VAT3(x, i, j+1, k)
00485                     + VAT3(oN, i, j-1, k) * VAT3(x, i, j-1, k)
00486                     + VAT3(oE, i, j, k) * VAT3(x, i+1, j, k)
00487                     + VAT3(oE, i-1, j, k) * VAT3(x, i-1, j, k)
00488                     + VAT3(uC, i, j, k-1) * VAT3(x, i, j, k-1)
00489                     + VAT3(uC, i, j, k) * VAT3(x, i, j, k+1)
00490                     - (VAT3(oC, i, j, k) + VAT3(cc, i, j, k)) * VAT3(x, i, j, k);
00491             }
00492         }
00493     }
00494 }
00495
00496
00497
00498 VPUBLIC void Vmresid27(int *nx, int *ny, int *nz,
00499     int *ipc, double *rpc,
00500     double *ac, double *cc, double *fc,
00501     double *x, double *r) {
00502
00503     MAT2(ac, *nx * *ny * *nz, 1);
00504
00505     // Do in one step
00506     Vmresid27_ls(nx,ny,nz,

```



```

00507         ipc, rpc,
00508         RAT2(ac, 1, 1),          cc,          fc,
00509         RAT2(ac, 1, 2), RAT2(ac, 1, 3), RAT2(ac, 1, 4),
00510         RAT2(ac, 1, 5), RAT2(ac, 1, 6),
00511         RAT2(ac, 1, 7), RAT2(ac, 1, 8), RAT2(ac, 1, 9), RAT2(ac, 1,10),
00512         RAT2(ac, 1,11), RAT2(ac, 1,12), RAT2(ac, 1,13), RAT2(ac, 1,14),
00513         x,r);
00514 }
00515
00516
00517
00518 VPUBLIC void Vmresid27_ls(int *nx, int *ny, int *nz,
00519 int *ipc, double *rpc,
00520 double *oC, double *cc, double *fc,
00521 double *oE, double *oN, double *uC,
00522 double *oNE, double *oNW,
00523 double *uE, double *uW, double *uN, double *uS,
00524 double *uNE, double *uNW, double *uSE, double *uSW,
00525 double *x, double *r) {
00526
00527     int i, j, k;
00528
00529     double tmpO, tmpU, tmpD;
00530
00531     MAT3(cc, *nx, *ny, *nz);
00532     MAT3(fc, *nx, *ny, *nz);
00533     MAT3(x, *nx, *ny, *nz);
00534     MAT3(r, *nx, *ny, *nz);
00535
00536     MAT3(oC, *nx, *ny, *nz);
00537     MAT3(oE, *nx, *ny, *nz);
00538     MAT3(oN, *nx, *ny, *nz);
00539     MAT3(oNE, *nx, *ny, *nz);
00540     MAT3(oNW, *nx, *ny, *nz);
00541
00542     MAT3(uC, *nx, *ny, *nz);
00543     MAT3(uE, *nx, *ny, *nz);
00544     MAT3(uW, *nx, *ny, *nz);
00545     MAT3(uN, *nx, *ny, *nz);
00546     MAT3(uS, *nx, *ny, *nz);
00547     MAT3(uNE, *nx, *ny, *nz);
00548     MAT3(uNW, *nx, *ny, *nz);
00549     MAT3(uSE, *nx, *ny, *nz);
00550     MAT3(uSW, *nx, *ny, *nz);
00551
00552     #pragma omp parallel for private(i, j, k, tmpO, tmpU, tmpD)
00553     for (k=2; k<=*nz-1; k++) {
00554         for (j=2; j<=*ny-1; j++) {
00555             for(i=2; i<=*nx-1; i++) {
00556
00557                 tmpO =
00558                     + VAT3( oN, i, j, k) * VAT3(x, i, j+1, k)
00559                     + VAT3( oN, i, j-1, k) * VAT3(x, i, j-1, k)
00560                     + VAT3( oE, i, j, k) * VAT3(x, i+1, j, k)
00561                     + VAT3( oE, i-1, j, k) * VAT3(x, i-1, j, k)
00562                     + VAT3( oNE, i, j, k) * VAT3(x, i+1, j+1, k)
00563                     + VAT3( oNW, i, j, k) * VAT3(x, i-1, j+1, k)
00564                     + VAT3( oNW, i+1, j-1, k) * VAT3(x, i+1, j-1, k)
00565                     + VAT3( oNE, i-1, j-1, k) * VAT3(x, i-1, j-1, k);
00566
00567                 tmpU =
00568                     + VAT3( uC, i, j, k) * VAT3(x, i, j, k+1)
00569                     + VAT3( uN, i, j, k) * VAT3(x, i, j+1, k+1)
00570                     + VAT3( uS, i, j, k) * VAT3(x, i, j-1, k+1)
00571                     + VAT3( uE, i, j, k) * VAT3(x, i+1, j, k+1)
00572                     + VAT3( uW, i, j, k) * VAT3(x, i-1, j, k+1)
00573                     + VAT3( uNE, i, j, k) * VAT3(x, i+1, j+1, k+1)
00574                     + VAT3( uNW, i, j, k) * VAT3(x, i-1, j+1, k+1)
00575                     + VAT3( uSE, i, j, k) * VAT3(x, i+1, j-1, k+1)
00576                     + VAT3( uSW, i, j, k) * VAT3(x, i-1, j-1, k+1);
00577
00578                 tmpD =
00579                     + VAT3( uC, i, j, k-1) * VAT3(x, i, j, k-1)
00580                     + VAT3( uS, i, j+1, k-1) * VAT3(x, i, j+1, k-1)
00581                     + VAT3( uN, i, j-1, k-1) * VAT3(x, i, j-1, k-1)
00582                     + VAT3( uW, i+1, j, k-1) * VAT3(x, i+1, j, k-1)
00583                     + VAT3( uE, i-1, j, k-1) * VAT3(x, i-1, j, k-1)
00584                     + VAT3( uSW, i+1, j+1, k-1) * VAT3(x, i+1, j+1, k-1)
00585                     + VAT3( uSE, i-1, j+1, k-1) * VAT3(x, i-1, j+1, k-1)
00586                     + VAT3( uNW, i+1, j-1, k-1) * VAT3(x, i+1, j-1, k-1)
00587                     + VAT3( uNE, i-1, j-1, k-1) * VAT3(x, i-1, j-1, k-1);

```

```

00588
00589         VAT3(r, i, j, k) = VAT3(fc, i, j, k) + tmpO + tmpU + tmpD
00590             - (VAT3(oC, i, j, k) + VAT3(cc, i, j, k)) * VAT3(x, i, j, k);
00591     }
00592 }
00593 }
00594 }
00595
00596
00597
00598 VPUBLIC void Vnmresid(int *nx, int *ny, int *nz,
00599     int *ipc, double *rpc,
00600     double *ac, double *cc, double *fc,
00601     double *x, double *r, double *w1) {
00602
00603     int numdia;
00604
00605     // Do in oNe step ***
00606     numdia = VAT(ipc, 11);
00607     if (numdia == 7) {
00608         Vnmresid7(nx, ny, nz, ipc, rpc, ac, cc, fc, x, r, w1);
00609     } else if (numdia == 27) {
00610         Vnmresid27(nx, ny, nz, ipc, rpc, ac, cc, fc, x, r, w1);
00611     } else {
00612         Vnm_print(2, "Vnmresid: invalid stencil type given...\n");
00613     }
00614 }
00615
00616
00617
00618 VPUBLIC void Vnmresid7(int *nx, int *ny, int *nz,
00619     int *ipc, double *rpc,
00620     double *ac, double *cc, double *fc,
00621     double *x, double *r, double *w1) {
00622
00623     MAT2(ac, *nx * *ny * *nz, 1);
00624
00625     // Do in oNe step
00626     Vnmresid7_ls(nx, ny, nz,
00627         ipc, rpc,
00628         RAT2(ac, 1, 1), cc, fc,
00629         RAT2(ac, 1, 2), RAT2(ac, 1, 3), RAT2(ac, 1, 4),
00630         x, r, w1);
00631 }
00632
00633 VPUBLIC void Vnmresid7_ls(int *nx, int *ny, int *nz,
00634     int *ipc, double *rpc,
00635     double *oC, double *cc, double *fc,
00636     double *oE, double *oN, double *uC,
00637     double *x, double *r, double *w1) {
00638
00639     int i, j, k;
00640     int ipkey;
00641
00642     MAT3(oE, *nx, *ny, *nz);
00643     MAT3(oN, *nx, *ny, *nz);
00644     MAT3(uC, *nx, *ny, *nz);
00645     MAT3(cc, *nx, *ny, *nz);
00646     MAT3(fc, *nx, *ny, *nz);
00647     MAT3(oC, *nx, *ny, *nz);
00648     MAT3(x, *nx, *ny, *nz);
00649     MAT3(r, *nx, *ny, *nz);
00650     MAT3(w1, *nx, *ny, *nz);
00651
00652     // First get vector nonlinear term to avoid subroutine calls
00653     ipkey = VAT(ipc, 10);
00654     Vc_vec(cc, x, w1, nx, ny, nz, &ipkey);
00655
00656     // The residual
00657     for (k=2; k<=*nz-1; k++) {
00658         for (j=2; j<=*ny-1; j++) {
00659             for (i=2; i<=*nx-1; i++) {
00660                 VAT3(r, i, j, k) = VAT3(fc, i, j, k)
00661                     + VAT3(oN, i, j, k) * VAT3(x, i, j+1, k)
00662                     + VAT3(oN, i, j-1, k) * VAT3(x, i, j-1, k)
00663                     + VAT3(oE, i, j, k) * VAT3(x, i+1, j, k)
00664                     + VAT3(oE, i-1, j, k) * VAT3(x, i-1, j, k)
00665                     + VAT3(uC, i, j, k-1) * VAT3(x, i, j, k-1)
00666                     + VAT3(uC, i, j, k) * VAT3(x, i, j, k+1)
00667                     - VAT3(oC, i, j, k) * VAT3(x, i, j, k)
00668                     - VAT3(w1, i, j, k);

```

```

00669     }
00670     }
00671 }
00672 }
00673
00674
00675
00676 VPUBLIC void Vnmresid27(int *nx, int *ny, int *nz,
00677     int *ipc, double *rpc,
00678     double *ac, double *cc, double *fc,
00679     double *x, double *r, double *w1) {
00680
00681     MAT2(ac, *nx * *ny * *nz, 1);
00682
00683     // Do in oNe step
00684     Vnmresid27_ls(nx, ny, nz,
00685         ipc, rpc,
00686         RAT2(ac, 1, 1), cc, fc,
00687         RAT2(ac, 1, 2), RAT2(ac, 1, 3), RAT2(ac, 1, 4),
00688         RAT2(ac, 1, 5), RAT2(ac, 1, 6),
00689         RAT2(ac, 1, 7), RAT2(ac, 1, 8), RAT2(ac, 1, 9), RAT2(ac, 1, 10),
00690         RAT2(ac, 1, 11), RAT2(ac, 1, 12), RAT2(ac, 1, 13), RAT2(ac, 1, 14),
00691         x, r, w1);
00692 }
00693
00694
00695
00696 VPUBLIC void Vnmresid27_ls(int *nx, int *ny, int *nz,
00697     int *ipc, double *rpc,
00698     double *oC, double *cc, double *fc,
00699     double *oE, double *oN, double *uC,
00700     double *oNE, double *oNW,
00701     double *uE, double *uW, double *uN, double *uS,
00702     double *uNE, double *uNW, double *uSE, double *uSW,
00703     double *x, double *r, double *w1) {
00704
00705     int i, j, k;
00706     int ipkey;
00707     double tmpO, tmpU, tmpD;
00708
00709     MAT3( oC, *nx, *ny, *nz);
00710     MAT3( cc, *nx, *ny, *nz);
00711     MAT3( fc, *nx, *ny, *nz);
00712     MAT3( oE, *nx, *ny, *nz);
00713     MAT3( oN, *nx, *ny, *nz);
00714     MAT3( uC, *nx, *ny, *nz);
00715     MAT3( oNE, *nx, *ny, *nz);
00716     MAT3( oNW, *nx, *ny, *nz);
00717     MAT3( uE, *nx, *ny, *nz);
00718     MAT3( uW, *nx, *ny, *nz);
00719     MAT3( uN, *nx, *ny, *nz);
00720     MAT3( uS, *nx, *ny, *nz);
00721     MAT3( uNE, *nx, *ny, *nz);
00722     MAT3( uNW, *nx, *ny, *nz);
00723     MAT3( uSE, *nx, *ny, *nz);
00724     MAT3( uSW, *nx, *ny, *nz);
00725     MAT3( x, *nx, *ny, *nz);
00726     MAT3( r, *nx, *ny, *nz);
00727     MAT3( w1, *nx, *ny, *nz);
00728
00729     // First get vector noNlinear term to avoid subroutine calls
00730     ipkey = VAT(ipc, 10);
00731     Vc_vec(cc, x, w1, nx, ny, nz, &ipkey);
00732
00733     // The residual
00734     for (k=2; k<=*nz-1; k++) {
00735         for (j=2; j<=*ny-1; j++) {
00736             for (i=2; i<=*nx-1; i++) {
00737
00738                 tmpO =
00739                     + VAT3( oN, i, j, k) * VAT3(x, i, j+1, k)
00740                     + VAT3( oN, i, j-1, k) * VAT3(x, i, j-1, k)
00741                     + VAT3( oE, i, j, k) * VAT3(x, i+1, j, k)
00742                     + VAT3( oE, i-1, j, k) * VAT3(x, i-1, j, k)
00743                     + VAT3( oNE, i, j, k) * VAT3(x, i+1, j+1, k)
00744                     + VAT3( oNW, i, j, k) * VAT3(x, i-1, j+1, k)
00745                     + VAT3( oNW, i+1, j-1, k) * VAT3(x, i+1, j-1, k)
00746                     + VAT3( oNE, i-1, j-1, k) * VAT3(x, i-1, j-1, k);
00747
00748                 tmpU =
00749                     + VAT3( uC, i, j, k) * VAT3(x, i, j, k+1)

```

```

00750         + VAT3( uN, i, j, k) * VAT3(x, i, j+1, k+1)
00751         + VAT3( uS, i, j, k) * VAT3(x, i, j-1, k+1)
00752         + VAT3( uE, i, j, k) * VAT3(x, i+1, j, k+1)
00753         + VAT3( uW, i, j, k) * VAT3(x, i-1, j, k+1)
00754         + VAT3( uNE, i, j, k) * VAT3(x, i+1, j+1, k+1)
00755         + VAT3( uNW, i, j, k) * VAT3(x, i-1, j+1, k+1)
00756         + VAT3( uSE, i, j, k) * VAT3(x, i+1, j-1, k+1)
00757         + VAT3( uSW, i, j, k) * VAT3(x, i-1, j-1, k+1);
00758
00759     tmpD =
00760         + VAT3( uC, i, j, k-1) * VAT3(x, i, j, k-1)
00761         + VAT3( uS, i, j+1, k-1) * VAT3(x, i, j+1, k-1)
00762         + VAT3( uN, i, j-1, k-1) * VAT3(x, i, j-1, k-1)
00763         + VAT3( uW, i+1, j, k-1) * VAT3(x, i+1, j, k-1)
00764         + VAT3( uE, i-1, j, k-1) * VAT3(x, i-1, j, k-1)
00765         + VAT3( uSW, i+1, j+1, k-1) * VAT3(x, i+1, j+1, k-1)
00766         + VAT3( uSE, i-1, j+1, k-1) * VAT3(x, i-1, j+1, k-1)
00767         + VAT3( uNW, i+1, j-1, k-1) * VAT3(x, i+1, j-1, k-1)
00768         + VAT3( uNE, i-1, j-1, k-1) * VAT3(x, i-1, j-1, k-1);
00769
00770     VAT3(r, i, j, k) =
00771         + tmpO + tmpU + tmpD
00772         + VAT3(fc, i, j, k)
00773         - VAT3(oC, i, j, k) * VAT3(x, i, j, k)
00774         - VAT3(w1, i, j, k);
00775     }
00776 }
00777 }
00778 }
00779
00780
00781
00782 VPUBLIC void Vrestrc(int *nxf, int *nyf, int *nzf,
00783     int *nxc, int *nyc, int *nzc,
00784     double *xin, double *xout, double *pc) {
00785
00786     MAT2(pc, *nxc * *nyc * *nzc, 1);
00787
00788     Vrestrc2(nxf, nyf, nzf,
00789         nxc, nyc, nzc,
00790         xin, xout,
00791         RAT2(pc, 1, 1), RAT2(pc, 1, 2), RAT2(pc, 1, 3), RAT2(pc, 1, 4), RAT2(pc, 1, 5),
00792         RAT2(pc, 1, 6), RAT2(pc, 1, 7), RAT2(pc, 1, 8), RAT2(pc, 1, 9),
00793         RAT2(pc, 1,10), RAT2(pc, 1,11), RAT2(pc, 1,12), RAT2(pc, 1,13), RAT2(pc, 1,14),
00794         RAT2(pc, 1,15), RAT2(pc, 1,16), RAT2(pc, 1,17), RAT2(pc, 1,18),
00795         RAT2(pc, 1,19), RAT2(pc, 1,20), RAT2(pc, 1,21), RAT2(pc, 1,22), RAT2(pc, 1,23),
00796         RAT2(pc, 1,24), RAT2(pc, 1,25), RAT2(pc, 1,26), RAT2(pc, 1,27));
00797 }
00798
00799
00800
00801 VEXTERNC void Vrestrc2(int *nxf, int *nyf, int *nzf,
00802     int *nxc, int *nyc, int *nzc,
00803     double *xin, double *xout,
00804     double *oPC, double *oPN, double *oPS, double *oPE, double *oPW,
00805     double *oPNE, double *oPNW, double *oPSE, double *oPSW,
00806     double *uPC, double *uPN, double *uPS, double *uPE, double *uPW,
00807     double *uPNE, double *uPNW, double *uPSE, double *uPSW,
00808     double *dPC, double *dPN, double *dPS, double *dPE, double *dPW,
00809     double *dPNE, double *dPNW, double *dPSE, double *dPSW) {
00810
00811     int i, j, k;
00812     int ii, jj, kk;
00813     int idimenshun = 3;
00814
00815     double tmpO, tmpU, tmpD;
00816     double dimfac;
00817
00818     MAT3(xin, *nxf, *nyf, *nzf);
00819     MAT3(xout, *nxc, *nyc, *nzc);
00820
00821     MAT3(oPC, *nxc, *nyc, *nzc);
00822     MAT3(oPN, *nxc, *nyc, *nzc);
00823     MAT3(oPS, *nxc, *nyc, *nzc);
00824     MAT3(oPE, *nxc, *nyc, *nzc);
00825     MAT3(oPW, *nxc, *nyc, *nzc);
00826
00827     MAT3(oPNE, *nxc, *nyc, *nzc);
00828     MAT3(oPNW, *nxc, *nyc, *nzc);
00829     MAT3(oPSE, *nxc, *nyc, *nzc);
00830     MAT3(oPSW, *nxc, *nyc, *nzc);

```

```

00831
00832     MAT3(uPC, *nxc, *nyc, *nzc);
00833     MAT3(uPN, *nxc, *nyc, *nzc);
00834     MAT3(uPS, *nxc, *nyc, *nzc);
00835     MAT3(uPE, *nxc, *nyc, *nzc);
00836     MAT3(uPW, *nxc, *nyc, *nzc);
00837
00838     MAT3(uPNE, *nxc, *nyc, *nzc);
00839     MAT3(uPNW, *nxc, *nyc, *nzc);
00840     MAT3(uPSE, *nxc, *nyc, *nzc);
00841     MAT3(uPSW, *nxc, *nyc, *nzc);
00842
00843     MAT3(dPC, *nxc, *nyc, *nzc);
00844     MAT3(dPN, *nxc, *nyc, *nzc);
00845     MAT3(dPS, *nxc, *nyc, *nzc);
00846     MAT3(dPE, *nxc, *nyc, *nzc);
00847     MAT3(dPW, *nxc, *nyc, *nzc);
00848
00849     MAT3(dPNE, *nxc, *nyc, *nzc);
00850     MAT3(dPNW, *nxc, *nyc, *nzc);
00851     MAT3(dPSE, *nxc, *nyc, *nzc);
00852     MAT3(dPSW, *nxc, *nyc, *nzc);
00853
00854     // Verify correctness of the input boundary points
00855     VfboundPMG00(nxf, nyf, nzf, xin);
00856
00857     dimfac = VPOW(2.0, idimenshun);
00858
00859     // Handle the interior points as average of 5 finer grid pts ***
00860     #pragma omp parallel for private(k, kk, j, jj, i, ii, tmpO, tmpU, tmpD)
00861     for (k=2; k<=*nzc-1; k++) {
00862         kk = (k - 1) * 2 + 1;
00863
00864         for (j=2; j<=*nyc-1; j++) {
00865             jj = (j - 1) * 2 + 1;
00866
00867             for (i=2; i<=*nxc-1; i++) {
00868                 ii = (i - 1) * 2 + 1;
00869
00870                 // Compute the restriction
00871                 tmpO =
00872                     + VAT3( oPC, i, j, k) * VAT3(xin, ii, jj, kk)
00873                     + VAT3( oPN, i, j, k) * VAT3(xin, ii, jj+1, kk)
00874                     + VAT3( oPS, i, j, k) * VAT3(xin, ii, jj-1, kk)
00875                     + VAT3( oPE, i, j, k) * VAT3(xin, ii+1, jj, kk)
00876                     + VAT3( oPW, i, j, k) * VAT3(xin, ii-1, jj, kk)
00877                     + VAT3( oPNE, i, j, k) * VAT3(xin, ii+1, jj+1, kk)
00878                     + VAT3( oPNW, i, j, k) * VAT3(xin, ii-1, jj+1, kk)
00879                     + VAT3( oPSE, i, j, k) * VAT3(xin, ii+1, jj-1, kk)
00880                     + VAT3( oPSW, i, j, k) * VAT3(xin, ii-1, jj-1, kk);
00881
00882                 tmpU =
00883                     + VAT3( uPC, i, j, k) * VAT3(xin, ii, jj, kk+1)
00884                     + VAT3( uPN, i, j, k) * VAT3(xin, ii, jj+1, kk+1)
00885                     + VAT3( uPS, i, j, k) * VAT3(xin, ii, jj-1, kk+1)
00886                     + VAT3( uPE, i, j, k) * VAT3(xin, ii+1, jj, kk+1)
00887                     + VAT3( uPW, i, j, k) * VAT3(xin, ii-1, jj, kk+1)
00888                     + VAT3( uPNE, i, j, k) * VAT3(xin, ii+1, jj+1, kk+1)
00889                     + VAT3( uPNW, i, j, k) * VAT3(xin, ii-1, jj+1, kk+1)
00890                     + VAT3( uPSE, i, j, k) * VAT3(xin, ii+1, jj-1, kk+1)
00891                     + VAT3( uPSW, i, j, k) * VAT3(xin, ii-1, jj-1, kk+1);
00892
00893                 tmpD =
00894                     + VAT3( dPC, i, j, k) * VAT3(xin, ii, jj, kk-1)
00895                     + VAT3( dPN, i, j, k) * VAT3(xin, ii, jj+1, kk-1)
00896                     + VAT3( dPS, i, j, k) * VAT3(xin, ii, jj-1, kk-1)
00897                     + VAT3( dPE, i, j, k) * VAT3(xin, ii+1, jj, kk-1)
00898                     + VAT3( dPW, i, j, k) * VAT3(xin, ii-1, jj, kk-1)
00899                     + VAT3( dPNE, i, j, k) * VAT3(xin, ii+1, jj+1, kk-1)
00900                     + VAT3( dPNW, i, j, k) * VAT3(xin, ii-1, jj+1, kk-1)
00901                     + VAT3( dPSE, i, j, k) * VAT3(xin, ii+1, jj-1, kk-1)
00902                     + VAT3( dPSW, i, j, k) * VAT3(xin, ii-1, jj-1, kk-1);
00903
00904                 VAT3(xout, i, j, k) = tmpO + tmpU + tmpD;
00905             }
00906         }
00907     }
00908
00909     // Verify correctness of the output boundary points
00910     VfboundPMG00(nxc, nyc, nzc, xout);
00911 }

```

```

00912
00913
00914
00915 VPUBLIC void VinterpPMG(int *nxc, int *nyc, int *nzc,
00916     int *nxf, int *nyf, int *nzf,
00917     double *xin, double *xout,
00918     double *pc) {
00919
00920     MAT2(pc, *nxc * *nyc * *nzc, 1);
00921
00922     VinterpPMG2(nxc, nyc, nzc,
00923         nxf, nyf, nzf,
00924         xin, xout,
00925         RAT2(pc, 1, 1), RAT2(pc, 1, 2), RAT2(pc, 1, 3), RAT2(pc, 1, 4), RAT2(pc, 1, 5),
00926         RAT2(pc, 1, 6), RAT2(pc, 1, 7), RAT2(pc, 1, 8), RAT2(pc, 1, 9),
00927         RAT2(pc, 1,10), RAT2(pc, 1,11), RAT2(pc, 1,12), RAT2(pc, 1,13), RAT2(pc, 1,14),
00928         RAT2(pc, 1,15), RAT2(pc, 1,16), RAT2(pc, 1,17), RAT2(pc, 1,18),
00929         RAT2(pc, 1,19), RAT2(pc, 1,20), RAT2(pc, 1,21), RAT2(pc, 1,22), RAT2(pc, 1,23),
00930         RAT2(pc, 1,24), RAT2(pc, 1,25), RAT2(pc, 1,26), RAT2(pc, 1,27));
00931 }
00932
00933
00934
00935 VPUBLIC void VinterpPMG2(int *nxc, int *nyc, int *nzc,
00936     int *nxf, int *nyf, int *nzf,
00937     double *xin, double *xout,
00938     double *oPC, double *oPN, double *oPS, double *oPE, double *oPW,
00939     double *oPNE, double *oPNW, double *oPSE, double *oPSW,
00940     double *uPC, double *uPN, double *uPS, double *uPE, double *uPW,
00941     double *uPNE, double *uPNW, double *uPSE, double *uPSW,
00942     double *dPC, double *dPN, double *dPS, double *dPE, double *dPW,
00943     double *dPNE, double *dPNW, double *dPSE, double *dPSW) {
00944
00945     int i, j, k;
00946     int ii, jj, kk;
00947
00948     MAT3( xin, *nxc, *nyc, *nzc);
00949     MAT3(xout, *nxf, *nyf, *nzf);
00950
00951     MAT3( oPC, *nxc, *nyc, *nzc);
00952     MAT3( oPN, *nxc, *nyc, *nzc);
00953     MAT3( oPS, *nxc, *nyc, *nzc);
00954     MAT3( oPE, *nxc, *nyc, *nzc);
00955     MAT3( oPW, *nxc, *nyc, *nzc);
00956
00957     MAT3(oPNE, *nxc, *nyc, *nzc);
00958     MAT3(oPNW, *nxc, *nyc, *nzc);
00959     MAT3(oPSE, *nxc, *nyc, *nzc);
00960     MAT3(oPSW, *nxc, *nyc, *nzc);
00961
00962     MAT3( uPC, *nxc, *nyc, *nzc);
00963     MAT3( uPN, *nxc, *nyc, *nzc);
00964     MAT3( uPS, *nxc, *nyc, *nzc);
00965     MAT3( uPE, *nxc, *nyc, *nzc);
00966     MAT3( uPW, *nxc, *nyc, *nzc);
00967
00968     MAT3(uPNE, *nxc, *nyc, *nzc);
00969     MAT3(uPNW, *nxc, *nyc, *nzc);
00970     MAT3(uPSE, *nxc, *nyc, *nzc);
00971     MAT3(uPSW, *nxc, *nyc, *nzc);
00972
00973     MAT3( dPC, *nxc, *nyc, *nzc);
00974     MAT3( dPN, *nxc, *nyc, *nzc);
00975     MAT3( dPS, *nxc, *nyc, *nzc);
00976     MAT3( dPE, *nxc, *nyc, *nzc);
00977     MAT3( dPW, *nxc, *nyc, *nzc);
00978
00979     MAT3(dPNE, *nxc, *nyc, *nzc);
00980     MAT3(dPNW, *nxc, *nyc, *nzc);
00981     MAT3(dPSE, *nxc, *nyc, *nzc);
00982     MAT3(dPSW, *nxc, *nyc, *nzc);
00983
00984     /* *****
00985     * Setup
00986     * *****
00987
00988     // Verify correctness of the input boundary points ***
00989     VfboundPMG00(nxc, nyc, nzc, xin);
00990
00991     // Do it
00992     for (k=1; k<=nzc-2; k+=2) {

```

```

00993     kk = (k - 1) / 2 + 1;
00994
00995     for (j=1; j<=nyf-2; j+=2) {
00996         jj = (j - 1) / 2 + 1;
00997
00998         for (i=1; i<=nxf-2; i+=2) {
00999             ii = (i - 1) / 2 + 1;
01000
01001             /* *****
01002              * Type 1 -- Fine grid points common to a coarse grid point *
01003              * ***** */
01004
01005             // Copy coinciding points from coarse grid to fine grid
01006             VAT3(xout, i, j, k) = VAT3(xin, ii, jj, kk);
01007
01008             /* *****
01009              * type 2 -- fine grid points common to a coarse grid plane *
01010              * ***** */
01011
01012             // Fine grid pts common only to y-z planes on coarse grid
01013             // (intermediate pts between 2 grid points on x-row)
01014             VAT3(xout, i+1, j, k) = VAT3(oPN, ii, jj, kk) * VAT3(xin, ii, jj, kk)
01015             + VAT3(oPW, ii+1, jj, kk) * VAT3(xin, ii+1, jj, kk);
01016
01017             // Fine grid pts common only to x-z planes on coarse grid
01018             // (intermediate pts between 2 grid points on a y-row)
01019             VAT3(xout, i, j+1, k) = VAT3(oPN, ii, jj, kk) * VAT3(xin, ii, jj, kk)
01020             + VAT3(oPS, ii, jj+1, kk) * VAT3(xin, ii, jj+1, kk);
01021
01022             // Fine grid pts common only to x-y planes on coarse grid
01023             // (intermediate pts between 2 grid points on a z-row)
01024             VAT3(xout, i, j, k+1) = VAT3(uPC, ii, jj, kk) * VAT3(xin, ii, jj, kk)
01025             + VAT3(dPC, ii, jj, kk+1) * VAT3(xin, ii, jj, kk+1);
01026
01027             /* *****
01028              * type 3 -- fine grid points common to a coarse grid line *
01029              * ***** */
01030
01031             // Fine grid pts common only to z planes on coarse grid
01032             // (intermediate pts between 4 grid pts on the xy-plane)
01033
01034             VAT3(xout, i+1, j+1, k) = VAT3(oPNE, ii, jj, kk) * VAT3(xin, ii, jj, kk)
01035             + VAT3(oPNW, ii+1, jj, kk) * VAT3(xin, ii+1, jj, kk)
01036             + VAT3(oPSE, ii, jj+1, kk) * VAT3(xin, ii, jj+1, kk)
01037             + VAT3(oPSW, ii+1, jj+1, kk) * VAT3(xin, ii+1, jj+1, kk);
01038
01039             // Fine grid pts common only to y planes on coarse grid
01040             // (intermediate pts between 4 grid pts on the xz-plane)
01041             VAT3(xout, i+1, j, k+1) = VAT3(uPE, ii, jj, kk) * VAT3(xin, ii, jj, kk)
01042             + VAT3(uPW, ii+1, jj, kk) * VAT3(xin, ii+1, jj, kk)
01043             + VAT3(dPE, ii, jj, kk+1) * VAT3(xin, ii, jj, kk+1)
01044             + VAT3(dPW, ii+1, jj, kk+1) * VAT3(xin, ii+1, jj, kk+1);
01045
01046             // Fine grid pts common only to x planes on coarse grid
01047             // (intermediate pts between 4 grid pts on the yz-plane)
01048             VAT3(xout, i, j+1, k+1) = VAT3(uPN, ii, jj, kk) * VAT3(xin, ii, jj, kk)
01049             + VAT3(uPS, ii, jj+1, kk) * VAT3(xin, ii, jj+1, kk)
01050             + VAT3(dPN, ii, jj, kk+1) * VAT3(xin, ii, jj, kk+1)
01051             + VAT3(dPS, ii, jj+1, kk+1) * VAT3(xin, ii, jj+1, kk+1);
01052
01053             /* *****
01054              * type 4 -- fine grid points not common to *
01055              * coarse grid pts/lines/planes *
01056              * ***** */
01057
01058             // Completely interior points
01059             VAT3(xout, i+1, j+1, k+1) =
01060                 + VAT3(uPNE, ii, jj, kk) * VAT3(xin, ii, jj, kk)
01061                 + VAT3(uPNW, ii+1, jj, kk) * VAT3(xin, ii+1, jj, kk)
01062                 + VAT3(uPSE, ii, jj+1, kk) * VAT3(xin, ii, jj+1, kk)
01063                 + VAT3(uPSW, ii+1, jj+1, kk) * VAT3(xin, ii+1, jj+1, kk)
01064                 + VAT3(dPNE, ii, jj, kk+1) * VAT3(xin, ii, jj, kk+1)
01065                 + VAT3(dPNW, ii+1, jj, kk+1) * VAT3(xin, ii+1, jj, kk+1)
01066                 + VAT3(dPSE, ii, jj+1, kk+1) * VAT3(xin, ii, jj+1, kk+1)
01067                 + VAT3(dPSW, ii+1, jj+1, kk+1) * VAT3(xin, ii+1, jj+1, kk+1);
01068         }
01069     }
01070 }
01071
01072 // Verify correctness of the output boundary points ***
01073 VfboundPMG00(nxf, nyf, nzf, xout);

```

```

01074 }
01075
01076
01077
01078 VPUBLIC void Vextrac(int *nxf, int *nyf, int *nzf,
01079 int *nxc, int *nyc, int *nzc,
01080 double *xin, double *xout) {
01081
01082     int i, j, k;
01083     int ii, jj, kk;
01084
01085     MAT3( xin, *nxf, *nyf, *nzf);
01086     MAT3(xout, *nxc, *nyc, *nzc);
01087
01088     // Verify correctness of the input boundary points
01089     VfboundPMG00(nxf, nyf, nzf, xin);
01090
01091     // Do it
01092     for (k=2; k<=*nzc-1; k++) {
01093         kk = (k - 1) * 2 + 1;
01094
01095         for (j=2; j<=*nyc-1; j++) {
01096             jj = (j - 1) * 2 + 1;
01097
01098             for (i=2; i<=*nxc-1; i++) {
01099                 ii = (i - 1) * 2 + 1;
01100
01101                 // Compute the restriction
01102                 VAT3(xout, i, j, k) = VAT3(xin, ii, jj, kk);
01103             }
01104         }
01105     }
01106
01107     // Verify correctness of the output boundary points
01108     VfboundPMG00(nxc, nyc, nzc, xout);
01109 }

```

9.127 matvecd.h

```

00001
00049 #ifndef _MATVECD_H_
00050 #define _MATVECD_H_
00051
00052 #include "apbscfg.h"
00053
00054 #include "generic/vhal.h"
00055 #include "generic/vmatrix.h"
00056 #include "pmgc/mikpckd.h"
00057 #include "pmgc/myppdec.h"
00058
00066 VEXTERNC void Vmatvec(
00067     int    *nx,
00068     int    *ny,
00069     int    *nz,
00070     int    *ipc,
00071     double *rpc,
00072     double *ac,
00073     double *cc,
00074     double *x,
00075     double *y
00076 );
00077
00078 VEXTERNC void Vmatvec7(
00079     int    *nx,
00080     int    *ny,
00081     int    *nz,
00082     int    *ipc,
00083     double *rpc,
00084     double *ac,
00085     double *cc,
00086     double *x,
00087     double *y
00088 );
00089
00090 VEXTERNC void Vmatvec7_ls(
00091     int    *nx,
00092     int    *ny,
00093     int    *nz,

```



```
00094         int      *ipc,
00095         double *rpc,
00096         double *oC,
00097         double *cc,
00098         double *oE,
00099         double *oN,
00100         double *uC,
00101         double *x,
00102         double *y
00103     );
00104
00105
00106
00107 VEXTERNC void Vmatvec27(
00108     int      *nx,
00109     int      *ny,
00110     int      *nz,
00111     int      *ipc,
00112     double *rpc,
00113     double *ac,
00114     double *cc,
00115     double *x,
00116     double *y
00117 );
00118
00119 VEXTERNC void Vmatvec27_1s(
00120     int      *nx,
00121     int      *ny,
00122     int      *nz,
00123     int      *ipc,
00124     double *rpc,
00125     double *oC,
00126     double *cc,
00127     double *oE,
00128     double *oN,
00129     double *uC,
00130     double *oNE,
00131     double *oNW,
00132     double *uE,
00133     double *uW,
00134     double *uN,
00135     double *uS,
00136     double *uNE,
00137     double *uNW,
00138     double *uSE,
00139     double *uSW,
00140     double *x,
00141     double *y
00142 );
00143
00144
00152 VEXTERNC void Vnmatvec(
00153     int *nx,
00154     int *ny,
00155     int *nz,
00156     int *ipc,
00157     double *rpc,
00158     double *ac,
00159     double *cc,
00160     double *x,
00161     double *y,
00162     double *wl
00163 );
00164
00165 VEXTERNC void Vnmatvec7(
00166     int      *nx,
00167     int      *ny,
00168     int      *nz,
00169     int      *ipc,
00170     double *rpc,
00171     double *ac,
00172     double *cc,
00173     double *x,
00174     double *y,
00175     double *wl
00176 );
00177
00178 VEXTERNC void Vnmatvecd7_1s(
00179     int      *nx,
00180     int      *ny,
00181     int      *nz,
```

```

00182         int      *ipc,
00183         double   *rpc,
00184         double   *oC,
00185         double   *cc,
00186         double   *oE,
00187         double   *oN,
00188         double   *uC,
00189         double   *x,
00190         double   *y,
00191         double   *wl
00192     );
00193
00194 VEXTERNC void Vnmatvec27(
00195     int      *nx,
00196     int      *ny,
00197     int      *nz,
00198     int      *ipc,
00199     double   *rpc,
00200     double   *ac,
00201     double   *cc,
00202     double   *x,
00203     double   *y,
00204     double   *wl
00205 );
00206
00207 VEXTERNC void Vnmatvecd27_1s(
00208     int      *nx,
00209     int      *ny,
00210     int      *nz,
00211     int      *ipc,
00212     double   *rpc,
00213     double   *oC,
00214     double   *cc,
00215     double   *oE,
00216     double   *oN,
00217     double   *uC,
00218     double   *oNE,
00219     double   *oNW,
00220     double   *uE,
00221     double   *uW,
00222     double   *uN,
00223     double   *uS,
00224     double   *uNE,
00225     double   *uNW,
00226     double   *uSE,
00227     double   *uSW,
00228     double   *x,
00229     double   *y,
00230     double   *wl
00231 );
00232
00233
00241 VEXTERNC void Vmresid(
00242     int      *nx,
00243     int      *ny,
00244     int      *nz,
00245     int      *ipc,
00246     double   *rpc,
00247     double   *ac,
00248     double   *cc,
00249     double   *fc,
00250     double   *x,
00251     double   *r
00252 );
00253
00254 VEXTERNC void Vmresid7(
00255     int      *nx,
00256     int      *ny,
00257     int      *nz,
00258     int      *ipc,
00259     double   *rpc,
00260     double   *ac,
00261     double   *cc,
00262     double   *fc,
00263     double   *x,
00264     double   *r
00265 );
00266
00267 VEXTERNC void Vmresid7_1s(
00268     int      *nx,
00269     int      *ny,

```

```
00270         int *nz,
00271         int *ipc,
00272         double *rpc,
00273         double *oC,
00274         double *cc,
00275         double *fc,
00276         double *oE,
00277         double *oN,
00278         double *uC,
00279         double *x,
00280         double *r
00281     );
00282
00283 VEXTERNC void Vmresid27(
00284     int *nx,
00285     int *ny,
00286     int *nz,
00287     int *ipc,
00288     double *rpc,
00289     double *ac,
00290     double *cc,
00291     double *fc,
00292     double *x,
00293     double *r
00294 );
00295
00296 VEXTERNC void Vmresid27_ls(
00297     int *nx,
00298     int *ny,
00299     int *nz,
00300     int *ipc,
00301     double *rpc,
00302     double *oC,
00303     double *cc,
00304     double *fc,
00305     double *oE,
00306     double *oN,
00307     double *uC,
00308     double *oNE,
00309     double *oNW,
00310     double *uE,
00311     double *uW,
00312     double *uN,
00313     double *uS,
00314     double *uNE,
00315     double *uNW,
00316     double *uSE,
00317     double *uSW,
00318     double *x,
00319     double *r
00320 );
00321
00322
00323
00331 VEXTERNC void Vnmresid(
00332     int *nx,
00333     int *ny,
00334     int *nz,
00335     int *ipc,
00336     double *rpc,
00337     double *ac,
00338     double *cc,
00339     double *fc,
00340     double *x,
00341     double *r,
00342     double *wl
00343 );
00344
00345 VEXTERNC void Vnmresid7(
00346     int *nx,
00347     int *ny,
00348     int *nz,
00349     int *ipc,
00350     double *rpc,
00351     double *ac,
00352     double *cc,
00353     double *fc,
00354     double *x,
00355     double *r,
00356     double *wl
00357 );
```

```
00358
00359 VEXTERNC void Vnmresid7_ls(
00360     int *nx,
00361     int *ny,
00362     int *nz,
00363     int *ipc,
00364     double *rpc,
00365     double *oC,
00366     double *cc,
00367     double *fc,
00368     double *oE,
00369     double *oN,
00370     double *uC,
00371     double *x,
00372     double *r,
00373     double *wl
00374 );
00375
00376 VEXTERNC void Vnmresid27(
00377     int *nx,
00378     int *ny,
00379     int *nz,
00380     int *ipc,
00381     double *rpc,
00382     double *ac,
00383     double *cc,
00384     double *fc,
00385     double *x,
00386     double *r,
00387     double *wl
00388 );
00389
00390 VEXTERNC void Vnmresid27_ls(
00391     int *nx,
00392     int *ny,
00393     int *nz,
00394     int *ipc,
00395     double *rpc,
00396     double *oC,
00397     double *cc,
00398     double *fc,
00399     double *oE,
00400     double *oN,
00401     double *uC,
00402     double *oNE,
00403     double *oNW,
00404     double *uE,
00405     double *uW,
00406     double *uN,
00407     double *uS,
00408     double *uNE,
00409     double *uNW,
00410     double *uSE,
00411     double *uSW,
00412     double *x,
00413     double *r,
00414     double *wl
00415 );
00416
00417
00418
00425 VEXTERNC void Vrestrc(
00426     int *nxf,
00427     int *nyf,
00428     int *nzf,
00429     int *nxc,
00430     int *nyc,
00431     int *nzc,
00432     double *xin,
00433     double *xout,
00434     double *pc
00435 );
00436
00437 VEXTERNC void Vrestrc2(
00438     int *nxf,
00439     int *nyf,
00440     int *nzf,
00441     int *nxc,
00442     int *nyc,
00443     int *nzc,
00444     double *xin,
```

```
00445         double *xout,
00446         double *oPC,
00447         double *oPN,
00448         double *oPS,
00449         double *oPE,
00450         double *oPW,
00451         double *oPNE,
00452         double *oPNW,
00453         double *oPSE,
00454         double *oPSW,
00455         double *uPC,
00456         double *uPN,
00457         double *uPS,
00458         double *uPE,
00459         double *uPW,
00460         double *uPNE,
00461         double *uPNW,
00462         double *uPSE,
00463         double *uPSW,
00464         double *dPC,
00465         double *dPN,
00466         double *dPS,
00467         double *dPE,
00468         double *dPW,
00469         double *dPNE,
00470         double *dPNW,
00471         double *dPSE,
00472         double *dPSW
00473     );
00474
00481 VEXTERNC void VinterpPMG(
00482     int     *nxc,
00483     int     *nyc,
00484     int     *nzc,
00485     int     *nxf,
00486     int     *nyf,
00487     int     *nzf,
00488     double *xin,
00489     double *xout,
00490     double *pc
00491 );
00492
00493 VEXTERNC void VinterpPMG2(
00494     int     *nxc,
00495     int     *nyc,
00496     int     *nzc,
00497     int     *nxf,
00498     int     *nyf,
00499     int     *nzf,
00500     double *xin,
00501     double *xout,
00502     double *oPC,
00503     double *oPN,
00504     double *oPS,
00505     double *oPE,
00506     double *oPW,
00507     double *oPNE,
00508     double *oPNW,
00509     double *oPSE,
00510     double *oPSW,
00511     double *uPC,
00512     double *uPN,
00513     double *uPS,
00514     double *uPE,
00515     double *uPW,
00516     double *uPNE,
00517     double *uPNW,
00518     double *uPSE,
00519     double *uPSW,
00520     double *dPC,
00521     double *dPN,
00522     double *dPS,
00523     double *dPE,
00524     double *dPW,
00525     double *dPNE,
00526     double *dPNW,
00527     double *dPSE,
00528     double *dPSW
00529 );
00530
00537 VEXTERNC void Vextrac(
```

```

00538         int *nxf,
00539         int *nyf,
00540         int *nzf,
00541         int *nxc,
00542         int *nyc,
00543         int *nzc,
00544         double *xin,
00545         double *xout
00546     );
00547
00548 #endif /* _MATVECD_H_ */

```

9.128 mgcsd.c

```

00001
00055 #include "mgcsd.h"
00056
00057 VEXTERN void Vmvecs(int *nx, int *ny, int *nz,
00058                     double *x,
00059                     int *iz,
00060                     double *w0, double *w1, double *w2, double *w3,
00061                     int *istop, int *itmax, int *iters, int *ierror,
00062                     int *nlev, int *ilev, int *nlev_real,
00063                     int *mgsolv, int *iok, int *iinfo,
00064                     double *epsiln, double *errtol, double *omega,
00065                     int *nul, int *nu2,
00066                     int *mgsmoo,
00067                     int *ipc, double *rpc,
00068                     double *pc, double *ac, double *cc, double *fc, double *tru) {
00069
00070     int level;          // @todo: doc
00071     int lev;            // @todo: doc
00072     int itmax_s;        // @todo: doc
00073     int iters_s;        // @todo: doc
00074     int nuu;            // @todo: doc
00075     int mgsmoo_s;       // @todo: doc
00076     int iresid;         // @todo: doc
00077     int nxf;            // @todo: doc
00078     int nyf;            // @todo: doc
00079     int nzf;            // @todo: doc
00080     int nxc;            // @todo: doc
00081     int nyc;            // @todo: doc
00082     int nzc;            // @todo: doc
00083     int lpv;            // @todo: doc
00084     int n;              // @todo: doc
00085     int m;              // @todo: doc
00086     int iadjoin;        // @todo: doc
00087     double errtol_s;    // @todo: doc
00088     double rsden;       // @todo: doc
00089     double rsnm;        // @todo: doc
00090     double orsnrm;      // @todo: doc
00091     double xnum;        // @todo: doc
00092     double xden;        // @todo: doc
00093     double xdamp;       // @todo: doc
00094     int lda;            // @todo: doc
00095
00096     double alpha;       // A utility variable used to pass a parameter to xaxpy
00097     int numlev;         // A utility variable used to pass a parameter to mkcors
00098
00099     MAT2(iz, 50, 1);
00100
00101     // Recover level information
00102     level = 1;
00103     lev = (*ilev - 1) + level;
00104
00105     // Recover grid sizes
00106     nxf = *nx;
00107     nyf = *ny;
00108     nzf = *nz;
00109     numlev = *nlev - 1;
00110     Vmkcors(&numlev, &nxf, &nyf, &nzf, &nxc, &nyc, &nzc);
00111
00112     // Do some i/o if requested
00113     if (*iinfo > 1) {
00114         VMESAGE0("Starting mvcs operation");
00115         VMESAGE3("Fine Grid Size: (%d, %d, %d)", nxf, nyf, nzf);
00116         VMESAGE3("Coarse Grid Size: (%d, %d, %d)", nxc, nyc, nzc);
00117     }

```

```

00118
00119     if (*iok != 0) {
00120         Vprtstp(*iok, -1, 0.0, 0.0, 0.0);
00121     }
00122 }
00123
00124 /* *****
00125  * *** Note: if (iok != 0) then: use a stopping test. ***
00126  * *** else: use just the itmax to stop iteration. ***
00127  * *****
00128  * *** istop=0 most efficient (whatever it is) ***
00129  * *** istop=1 relative residual ***
00130  * *** istop=2 rms difference of successive iterates ***
00131  * *** istop=3 relative true error (provided for testing) ***
00132  * *****/
00133
00134 // Compute denominator for stopping criterion
00135 if (*iok != 0) {
00136     if (*istop == 0) {
00137         rsden = 1.0;
00138     }
00139     else if (*istop == 1) {
00140         rsden = Vxnorm1(&nxf, &nyf, &nzf, RAT(fc, VAT2(iz, 1,lev)));
00141     }
00142     else if (*istop == 2) {
00143         rsden = VSQRT(nxf * nyf * nzf);
00144     }
00145     else if (*istop == 3) {
00146         rsden = Vxnorm2(&nxf, &nyf, &nzf, RAT(tru, VAT2(iz, 1,lev)));
00147     }
00148     else if (*istop == 4) {
00149         rsden = Vxnorm2(&nxf, &nyf, &nzf, RAT(tru, VAT2(iz, 1,lev)));
00150     }
00151     else if (*istop == 5) {
00152         Vmatvec(&nxf, &nyf, &nzf,
00153             RAT(ipc, VAT2(iz, 5,lev)), RAT(rpc, VAT2(iz, 6,lev)),
00154             RAT(ac, VAT2(iz, 7,lev)), RAT(cc, VAT2(iz, 1,lev)),
00155             RAT(tru, VAT2(iz, 1,lev)), w1);
00156         rsden = VSQRT(Vxdot(&nxf, &nyf, &nzf, RAT(tru, VAT2(iz, 1,lev)), w1));
00157     }
00158     else {
00159         VABORT_MSG1("Bad istop value: %d", *istop);
00160     }
00161
00162     if (rsden == 0.0) {
00163         rsden = 1.0;
00164         VERRMSG0("rhs is zero on finest level");
00165     }
00166     rsnorm = rsden;
00167     orsnrm = rsnorm;
00168     iters_s = 0;
00169
00170     Vprtstp(*iok, 0, rsnorm, rsden, orsnrm);
00171 }
00172
00173
00174
00175 /* *****
00176  * *** solve directly if nlev = 1 ***
00177  * *****/
00178
00179 // Solve directly if on the coarse grid
00180 if (*nlev == 1) {
00181
00182     // Use iterative method?
00183     if (*mgsolv == 0) {
00184
00185         // solve on coarsest grid with cgls, mgsmoo_s=4 (no residual)
00186         iresid = 0;
00187         iadjoin = 0;
00188         itmax_s = 100;
00189         iters_s = 0;
00190         errtol_s = *epsiln;
00191         mgsmoo_s = 4;
00192
00193         Vazeros(&nxf, &nyf, &nzf, RAT(x, VAT2(iz, 1,lev)));
00194
00195         Vsmooth(&nxf, &nyf, &nzf,
00196             RAT(ipc, VAT2(iz, 5,lev)), RAT(rpc, VAT2(iz, 6,lev)),
00197             RAT(ac, VAT2(iz, 7,lev)), RAT(cc, VAT2(iz, 1,lev)), RAT(fc, VAT2(iz, 1,lev)),
00198             RAT(x, VAT2(iz, 1,lev)), w1, w2, w3,

```

```

00199             &itmax_s, &iters_s, &errtol_s, omega,
00200             &iresid, &iadjoin, &mgsmoos);
00201
00202         // Check for trouble on the coarse grid
00203         VWARN_MSG2(iters_s <= itmax_s,
00204             "Exceeded maximum iterations: iters_s=%d, itmax_s=%d",
00205             iters_s, itmax_s);
00206
00207     } else if (*mgsolv == 1) {
00208
00209         // Use direct method?
00210
00211         // Setup lpv to access the factored/banded operator
00212         lpv = lev + 1;
00213
00214         // setup for banded format
00215         n = *RAT(ipc, (VAT2(iz, 5,lpv) - 1) + 1);
00216         m = *RAT(ipc, (VAT2(iz, 5,lpv) - 1) + 2);
00217         lda = *RAT(ipc, (VAT2(iz, 5,lpv) - 1) + 3);
00218
00219         // Call dpbsl to solve
00220         Vxcopy_small(&nxf, &nyf, &nzf, RAT(fc, VAT2(iz, 1,lev)), wl);
00221         Vdpbsl(RAT(ac, VAT2(iz, 7,lpv)), &lda, &n, &m, wl);
00222         Vxcopy_large(&nxf, &nyf, &nzf, wl, RAT(x, VAT2(iz, 1,lev)));
00223         VfboundPMG00(&nxf, &nyf, &nzf, RAT(x, VAT2(iz, 1,lev)));
00224
00225     } else {
00226         VABORT_MSG1("Invalid coarse solver requested: %d", *mgsolv);
00227     }
00228
00229     // Compute the stopping test
00230     *iters = 1;
00231     if (*iok != 0) {
00232         orsnrm = rsnm;
00233
00234         if (*istop == 0) {
00235
00236             Vmresid(&nxf, &nyf, &nzf,
00237                 RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00238                 RAT( ac, VAT2(iz, 7, lev)), RAT(cc , VAT2(iz, 1, lev)),
00239                 RAT( fc, VAT2(iz, 1,lev)),
00240                 RAT( x, VAT2(iz, 1, lev)), wl);
00241
00242             rsnm = Vxnrm1(&nxf, &nyf, &nzf, wl);
00243         }
00244
00245         else if (*istop == 1) {
00246
00247             Vmresid(&nxf, &nyf, &nzf,
00248                 RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00249                 RAT( ac, VAT2(iz, 7, lev)), RAT( cc, VAT2(iz, 1, lev)),
00250                 RAT( fc, VAT2(iz, 1, lev)), RAT( x, VAT2(iz, 1, lev)),
00251                 wl);
00252             rsnm = Vxnrm1(&nxf, &nyf, &nzf, wl);
00253         }
00254
00255         else if (*istop == 2) {
00256
00257             alpha = -1.0;
00258
00259             Vxcopy(&nxf, &nyf, &nzf, RAT(tru, VAT2(iz, 1,lev)), wl);
00260             Vxaxpy(&nxf, &nyf, &nzf, &alpha,
00261                 RAT(x, VAT2(iz, 1,lev)), wl);
00262             rsnm = Vxnrm1(&nxf, &nyf, &nzf, wl);
00263             Vxcopy(&nxf, &nyf, &nzf, RAT(x, VAT2(iz, 1,lev)), RAT(tru, VAT2(iz, 1,lev)));
00264         }
00265
00266         else if (*istop == 3) {
00267
00268             alpha = -1.0;
00269
00270             Vxcopy(&nxf, &nyf, &nzf, RAT(tru, VAT2(iz, 1,lev)), wl);
00271             Vxaxpy(&nxf, &nyf, &nzf, &alpha, RAT(x, VAT2(iz, 1,lev)), wl);
00272             rsnm = Vxnrm2(&nxf, &nyf, &nzf, wl);
00273         }
00274
00275         else if (*istop == 4) {
00276
00277             alpha = -1.0;

```



```

00280
00281     Vxcopy(&nxf, &nyf, &nzf, RAT(tru, VAT2(iz, 1,lev)), w1);
00282     Vxaxy(&nxf, &nyf, &nzf, &alpha, RAT(x, VAT2(iz, 1,lev)), w1);
00283     rsnrm = Vxnm2(&nxf, &nyf, &nzf, w1);
00284 }
00285
00286 else if (*istop == 5) {
00287     alpha = -1.0;
00288
00289     Vxcopy(&nxf, &nyf, &nzf, RAT(tru, VAT2(iz, 1,lev)), w1);
00290     Vxaxy(&nxf, &nyf, &nzf, &alpha, RAT(x, VAT2(iz, 1,lev)), w1);
00291
00292     Vmatvec(&nxf, &nyf, &nzf,
00293             RAT(ipc, VAT2(iz, 5,lev)), RAT(rpc, VAT2(iz, 6,lev)),
00294             RAT(ac, VAT2(iz, 7,lev)), RAT(cc, VAT2(iz, 1,lev)),
00295             w1, w2);
00296     rsnrm = VSQRT(Vxdot(&nxf, &nyf, &nzf, w1, w2));
00297 }
00298
00299 else {
00300     VABORT_MSG1("Bad istop value: %d\n", *istop);
00301 }
00302 Vprtstp(*iok, *iters, rsnrm, rsden, orsnrm);
00303 }
00304 return;
00305 }
00306
00307
00308
00309 /* *****
00310  * *** begin mg iteration (note nxf,nyf,nzf changes during loop)
00311  * *****/
00312
00313 // Setup for the v-cycle looping
00314 *iters = 0;
00315 do {
00316     // Finest level initialization
00317     level = 1;
00318     lev = (*ilev - 1) + level;
00319
00320     // nul pre-smoothings on fine grid (with residual)
00321     iresid = 1;
00322     iadjoint = 0;
00323     iters_s = 0;
00324     errtol_s = 0.0;
00325     nuu = Vivariv(nul, &lev);
00326
00327     Vsmooth(&nxf, &nyf, &nzf,
00328             RAT(ipc, VAT2(iz, 5,lev)), RAT(rpc, VAT2(iz, 6,lev)),
00329             RAT(ac, VAT2(iz, 7,lev)), RAT(cc, VAT2(iz, 1,lev)), RAT(fc, VAT2(iz, 1,lev)),
00330             RAT(x, VAT2(iz, 1,lev)), w2, w3, w1,
00331             &nuu, &iters_s,
00332             &errtol_s, omega,
00333             &iresid, &iadjoint, mgsmoo);
00334
00335     Vxcopy(&nxf, &nyf, &nzf, w1, RAT(w0, VAT2(iz, 1,lev)));
00336
00337
00338
00339
00340 /* *****
00341  * begin cycling down to coarse grid
00342  * *****/
00343
00344 // Go down grids: restrict resid to coarser and smooth
00345 for (level=2; level<=nlev; level++) {
00346     lev = (*ilev - 1) + level;
00347
00348     // Find new grid size
00349     numlev = 1;
00350     Vmkcors(&numlev, &nxf, &nyf, &nzf, &nxc, &nyc, &nzc);
00351
00352     // Restrict residual to coarser grid ***
00353     Vrestrc(&nxf, &nyf, &nzf,
00354             &nxc, &nyc, &nzc,
00355             w1, RAT(w0, VAT2(iz, 1,lev)), RAT(pc, VAT2(iz, 11,lev-1)));
00356
00357     nxf = nxc;
00358     nyf = nyc;
00359     nzf = nzc;
00360
00361

```

```

00362
00363 // if not on coarsest level yet...
00364 if (level != *nlev) {
00365
00366     // nul pre-smoothings on this level (with residual)
00367     // (w1 has residual...)
00368     Vazeros(&nxf, &nyf, &nzf, RAT(x, VAT2(iz, 1,lev)));
00369     iresid = 1;
00370     iadjoint = 0;
00371     iters_s = 0;
00372     errtol_s = 0.0;
00373     nuuu = Vivariv(nul, &lev);
00374     Vsmooth(&nxf, &nyf, &nzf,
00375             RAT(ipc, VAT2(iz, 5,lev)), RAT(rpc, VAT2(iz, 6,lev)),
00376             RAT(ac, VAT2(iz, 7,lev)), RAT(cc, VAT2(iz, 1,lev)), RAT(w0, VAT2(iz, 1,lev)),
00377             RAT(x, VAT2(iz, 1,lev)), w2, w3, w1,
00378             &nuuu, &iters_s,
00379             &errtol_s, omega,
00380             &iresid, &iadjoint, mgsmoo);
00381 }
00382 // End of cycling down to coarse grid loop
00383 }
00384
00385
00386
00387 /* *****
00388 * begin coarse grid
00389 * *****
00390
00391 // Coarsest level
00392 level = *nlev;
00393 lev = (*ilev - 1) + level;
00394
00395 // Use iterative method?
00396 if (*mgsolv == 0) {
00397
00398     // solve on coarsest grid with cghs, mgsmoo_s=4 (no residual)
00399     iresid = 0;
00400     iadjoint = 0;
00401     itmax_s = 100;
00402     iters_s = 0;
00403     errtol_s = *epsiln;
00404     mgsmoo_s = 4;
00405     Vazeros(&nxf, &nyf, &nzf, RAT(x, VAT2(iz, 1,lev)));
00406     Vsmooth(&nxf, &nyf, &nzf,
00407             RAT(ipc, VAT2(iz, 5,lev)), RAT(rpc, VAT2(iz, 6,lev)),
00408             RAT(ac, VAT2(iz, 7,lev)), RAT(cc, VAT2(iz, 1,lev)), RAT(w0, VAT2(iz, 1,lev)),
00409             RAT(x, VAT2(iz, 1,lev)), w1, w2, w3,
00410             &itmax_s, &iters_s,
00411             &errtol_s, omega,
00412             &iresid, &iadjoint, &mgsmoo_s);
00413
00414     // Check for trouble on the coarse grid
00415     VWARN_MSG2(iters_s <= itmax_s,
00416               "Exceeded maximum iterations: iters_s=%d, itmax_s=%d",
00417               iters_s, itmax_s);
00418 } else if (*mgsolv == 1) {
00419
00420     // use direct method?
00421
00422     // Setup lpv to access the factored/banded operator
00423     lpv = lev + 1;
00424
00425     // Setup for banded format
00426     n = VAT(ipc, (VAT2(iz, 5, lpv) - 1) + 1);
00427     m = VAT(ipc, (VAT2(iz, 5, lpv) - 1) + 2);
00428     lda = VAT(ipc, (VAT2(iz, 5, lpv) - 1) + 3);
00429
00430     // Call dpbsl to solve
00431     Vxcopy_small(&nxf, &nyf, &nzf, RAT(w0, VAT2(iz, 1,lev)), w1);
00432     Vdpbsl(RAT(ac, VAT2(iz, 7,lpv)), &lda, &n, &m, w1);
00433     Vxcopy_large(&nxf, &nyf, &nzf, w1, RAT(x, VAT2(iz, 1,lev)));
00434     VfboundPMG00(&nxf, &nyf, &nzf, RAT(x, VAT2(iz, 1,lev)));
00435
00436 } else {
00437     VABORT_MSG1("Invalid coarse solver requested: %d", *mgsolv);
00438 }
00439
00440
00441 /* *****
00442 * begin cycling back to fine grid

```

```

00443      * *****/
00444
00445
00446      // Move up grids: interpolate resid to finer and smooth
00447      for (level=nnlev-1; level>=1; level--) {
00448
00449          lev = (*ilev - 1) + level;
00450
00451          // Find new grid size
00452          numlev = 1;
00453          Vmkfine(&numlev,
00454                &nxf, &nyf, &nzf,
00455                &nxc, &nyc, &nzc);
00456
00457          // Interpolate to next finer grid
00458          VinterpPMG(&nxf, &nyf, &nzf,
00459                   &nxc, &nyc, &nzc,
00460                   RAT(x, VAT2(iz, 1,lev+1)), w1, RAT(pc, VAT2(iz, 11,lev)));
00461
00462          /* Compute the hackbusch/reusken damping parameter
00463           * which is equivalent to the standard linear cg steplength
00464           */
00465          Vmatvec(&nxf, &nyf, &nzf,
00466                RAT(ipc, VAT2(iz, 5,lev+1)), RAT(rpc, VAT2(iz, 6,lev+1)),
00467                RAT(ac, VAT2(iz, 7,lev+1)), RAT(cc, VAT2(iz, 1,lev+1)),
00468                RAT(x, VAT2(iz, 1,lev+1)), w2);
00469
00470          xnum = Vxdot(&nxf, &nyf, &nzf,
00471                    RAT(x, VAT2(iz, 1,lev+1)), RAT(w0, VAT2(iz, 1,lev+1)));
00472
00473          xden = Vxdot(&nxf, &nyf, &nzf,
00474                    RAT(x, VAT2(iz, 1,lev+1)), w2);
00475          xdamp = xnum / xden;
00476
00477          // New grid size
00478          nxf = nxc;
00479          nyf = nyc;
00480          nzf = nzc;
00481
00482          // perform the coarse grid correction
00483          // xdamp = 1.0d0
00484          Vxaxpy(&nxf, &nyf, &nzf,
00485                &xdamp, w1, RAT(x, VAT2(iz, 1,lev)));
00486
00487          // nu2 post-smoothings for correction (no residual)
00488          iresid = 0;
00489          iadjoin = 1;
00490          iters_s = 0;
00491          errtol_s = 0.0;
00492          nuuu = Vivariv(nu2, &lev);
00493          if (level == 1) {
00494              Vsmooth(&nxf, &nyf, &nzf,
00495                    RAT(ipc, VAT2(iz, 5,lev)), RAT(rpc, VAT2(iz, 6,lev)),
00496                    RAT(ac, VAT2(iz, 7,lev)), RAT(cc, VAT2(iz, 1,lev)), RAT(fc, VAT2(iz, 1,lev)),
00497                    RAT(x, VAT2(iz, 1,lev)), w1, w2, w3,
00498                    &nuuu, &iters_s, &errtol_s, omega,
00499                    &iresid, &iadjoin, mgsmoo);
00500          } else {
00501              Vsmooth(&nxf, &nyf, &nzf,
00502                    RAT(ipc, VAT2(iz, 5,lev)), RAT(rpc, VAT2(iz, 6,lev)),
00503                    RAT(ac, VAT2(iz, 7,lev)), RAT(cc, VAT2(iz, 1,lev)), RAT(w0, VAT2(iz, 1,lev)),
00504                    RAT(x, VAT2(iz, 1,lev)), w1, w2, w3,
00505                    &nuuu, &iters_s, &errtol_s, omega,
00506                    &iresid, &iadjoin, mgsmoo);
00507          }
00508      }
00509
00510      /* *****/
00511      * iteration complete: do some i/o
00512      * *****/
00513
00514      // Increment the iteration counter
00515      (*iters)++;
00516
00517      // Compute/check the current stopping test
00518      if (iok != 0) {
00519          orsnrm = rsnrm;
00520          if (*istop == 0) {
00521              Vmresid(&nxf, &nyf, &nzf,
00522                    RAT(ipc, VAT2(iz, 5,lev)), RAT(rpc, VAT2(iz, 6,lev)),
00523                    RAT(ac, VAT2(iz, 7,lev)), RAT(cc, VAT2(iz, 1,lev)), RAT(fc, VAT2(iz, 1,lev)),

```

```

00524         RAT(x, VAT2(iz, 1,lev)), w1);
00525         rsnm = Vxnm1(&nxf, &nyf, &nzf, w1);
00526     } else if(*istop == 1) {
00527         Vmresid(&nxf, &nyf, &nzf,
00528             RAT(ipc, VAT2(iz, 5,lev)), RAT(rpc, VAT2(iz, 6,lev)),
00529             RAT(ac, VAT2(iz, 7,lev)), RAT(cc, VAT2(iz, 1,lev)), RAT(fc, VAT2(iz, 1,lev)),
00530             RAT(x, VAT2(iz, 1,lev)), w1);
00531         rsnm = Vxnm1(&nxf, &nyf, &nzf, w1);
00532     } else if (*istop == 2) {
00533         Vxcopy(&nxf, &nyf, &nzf, RAT(tru, VAT2(iz, 1,lev)), w1);
00534         alpha = -1.0;
00535         Vxaxy(&nxf, &nyf, &nzf, &alpha, RAT(x, VAT2(iz, 1,lev)), w1);
00536         rsnm = Vxnm1(&nxf, &nyf, &nzf, w1);
00537         Vxcopy(&nxf, &nyf, &nzf, RAT(x, VAT2(iz, 1,lev)), RAT(tru, VAT2(iz, 1,lev)));
00538     } else if (*istop == 3) {
00539         Vxcopy(&nxf, &nyf, &nzf, RAT(tru, VAT2(iz, 1,lev)), w1);
00540         alpha = -1.0;
00541         Vxaxy(&nxf, &nyf, &nzf, &alpha, RAT(x, VAT2(iz, 1,lev)), w1);
00542         rsnm = Vxnm2(&nxf, &nyf, &nzf, w1);
00543     } else if (*istop == 4) {
00544         Vxcopy(&nxf, &nyf, &nzf, RAT(tru, VAT2(iz, 1,lev)), w1);
00545         alpha = -1.0;
00546         Vxaxy(&nxf, &nyf, &nzf, &alpha, RAT(x, VAT2(iz, 1,lev)), w1);
00547         rsnm = Vxnm2(&nxf, &nyf, &nzf, w1);
00548     } else if (*istop == 5) {
00549         Vxcopy(&nxf, &nyf, &nzf, RAT(tru, VAT2(iz, 1,lev)), w1);
00550         alpha = -1.0;
00551         Vxaxy(&nxf, &nyf, &nzf, &alpha, RAT(x, VAT2(iz, 1,lev)), w1);
00552         Vmatvec(&nxf, &nyf, &nzf,
00553             RAT(ipc, VAT2(iz, 5,lev)), RAT(rpc, VAT2(iz, 6,lev)),
00554             RAT(ac, VAT2(iz, 7,lev)), RAT(cc, VAT2(iz, 1,lev)),
00555             w1, w2);
00556         rsnm = VSQRT(Vxdot(&nxf, &nyf, &nzf, w1, w2));
00557     } else {
00558         VABORT_MSG1("Bad istop value: %d", *istop);
00559     }
00560     Vprtstp(*iok, *iters, rsnm, rsden, orsnm);
00561 }
00562 } while (*iters<*itmax && (rsnm/rsden) > *errtol);
00563
00564 *ierror = *iters < *itmax ? 0 : 1;
00565 }

```

9.129 mgcsd.h

```

00001
00050 #ifndef _MGCSH_H_
00051 #define _MGCSH_H_
00052
00053 #include "apbscfg.h"
00054
00055 #include "malloc/malloc.h"
00056
00057 #include "generic/vhal.h"
00058 #include "generic/vmatrix.h"
00059 #include "pmgc/mgsubd.h"
00060 #include "pmgc/mikpckd.h"
00061 #include "pmgc/smoothd.h"
00062 #include "pmgc/gsd.h"
00063 #include "pmgc/matvecd.h"
00064 #include "pmgc/mlinpckd.h"
00065
00106 VEXTERN void Vmvs(
00107     int    nx,
00108     int    ny,
00109     int    nz,
00110     double x,
00111     int    iz,
00112     double w0,
00113     double w1,
00114     double w2,
00115     double w3,
00116     int    istop,
00117     int    itmax,
00118     int    iters,
00119     int    ierror,
00120     int    nlev,
00121     int    ilev,

```

```

00122         int      *nlev_real,
00123         int      *mgsolv,
00124         int      *iok,
00125         int      *iinfo,
00126         double   *epsiln,
00127         double   *errtol,
00128         double   *omega,
00129         int      *nu1,
00130         int      *nu2,
00131         int      *mgsmoo,
00132         int      *ipc,
00133         double   *rpc,
00134         double   *pc,
00135         double   *ac,
00136         double   *cc,
00137         double   *fc,
00138         double   *tru
00139     );
00140
00141 #endif /* _MGCSD_H_ */

```

9.130 mgdrvd.c

```

00001
00055 #include "mgdrvd.h"
00056
00057 VPUBLIC void Vmgdriv(int* iparm, double* rparm,
00058     int* iwork, double* rwork, double* u,
00059     double* xf, double* yf, double* zf,
00060     double* gxcf, double* gycf, double* gzcf,
00061     double* alcf, double* a2cf, double* a3cf,
00062     double* ccf, double* fcf, double* tcf) {
00063
00064     // The following variables will be returned from mgsz
00065     int nxc = 0;
00066     int nyc = 0;
00067     int nzc = 0;
00068     int nf = 0;
00069     int nc = 0;
00070     int narr = 0;
00071     int narrc = 0;
00072     int n_rpc = 0;
00073     int n_iz = 0;
00074     int n_ipc = 0;
00075     int iretot = 0;
00076     int iintot = 0;
00077
00078     // Miscellaneous variables
00079     int nrwk = 0;
00080     int niwk = 0;
00081     int nx = 0;
00082     int ny = 0;
00083     int nz = 0;
00084     int nlev = 0;
00085     int ierror = 0;
00086     int mxlv = 0;
00087     int mgcoar = 0;
00088     int mgdisc = 0;
00089     int mgsolv = 0;
00090     int k_iz = 0;
00091     int k_ipc = 0;
00092     int k_rpc = 0;
00093     int k_ac = 0;
00094     int k_cc = 0;
00095     int k_fc = 0;
00096     int k_pc = 0;
00097
00098     // Utility pointers to help in passing values
00099     int *iz = VNULL;
00100     int *ipc = VNULL;
00101     double *rpc = VNULL;
00102     double *pc = VNULL;
00103     double *ac = VNULL;
00104     double *cc = VNULL;
00105     double *fc = VNULL;
00106
00107     // Decode some parameters
00108     nrwk = VAT(iparm, 1);

```

```

00109     niwk  = VAT(iparm, 2);
00110     nx    = VAT(iparm, 3);
00111     ny    = VAT(iparm, 4);
00112     nz    = VAT(iparm, 5);
00113     nlev  = VAT(iparm, 6);
00114
00115     // Perform some checks on input
00116     VASSERT_MSG1(nlev > 0, "nlev must be positive: %d", nlev);
00117     VASSERT_MSG1( nx > 0, "nx must be positive: %d", nx);
00118     VASSERT_MSG1( ny > 0, "ny must be positive: %d", ny);
00119     VASSERT_MSG1( nz > 0, "nz must be positive: %d", nz);
00120
00121     mxlv = Vmaxlev(nx, ny, nz);
00122     VASSERT_MSG2(
00123         nlev <= mxlv,
00124         "number of levels exceeds maximum: %d > %d",
00125         nlev, mxlv
00126     );
00127
00128
00129     // Extract basic grid sizes, etc.
00130     mgcoar = VAT(iparm, 18);
00131     mgdisc = VAT(iparm, 19);
00132     mgsolv = VAT(iparm, 21);
00133
00134     Vmgsz(&mgcoar, &mgdisc, &mgsolv,
00135          &nx, &ny, &nz,
00136          &nlev,
00137          &nxc, &nyc, &nzc,
00138          &nf, &nc,
00139          &narr, &narrc,
00140          &n_rpc, &n_iz, &n_ipc,
00141          &ioretot, &iintot);
00142
00143     // Perform some more checks on input
00144     VASSERT_MSG2(
00145         ioretot >= nrwk,
00146         "real workspace exceeds maximum size: %d > %d",
00147         nrwk, ioretot
00148     );
00149     VASSERT_MSG2(
00150         iintot >= niwk,
00151         "integer workspace exceeds maximum size: %d > %d",
00152         niwk, iintot
00153     );
00154
00155     // Split up the integer work array
00156     k_iz = 1;
00157     k_ipc = k_iz + n_iz;
00158
00159     // Split up the real work array ***
00160     k_rpc = 1;
00161     k_cc  = k_rpc + n_rpc;
00162     k_fc  = k_cc  + narr;
00163     k_pc  = k_fc  + narr;
00164     k_ac  = k_pc  + 27 * narrc;
00165     // k_ac_after = 4 * nf + 4 * narrc;
00166     // k_ac_after = 4 * nf + 14 * narrc;
00167     // k_ac_after = 14 * nf + 14 * narrc;
00168
00169     iz = RAT(iwork, k_iz);
00170     ipc = RAT(iwork, k_ipc);
00171
00172     rpc = RAT(rwork, k_rpc);
00173     pc  = RAT(rwork, k_pc);
00174     ac  = RAT(rwork, k_ac);
00175     cc  = RAT(rwork, k_cc);
00176     fc  = RAT(rwork, k_fc);
00177
00178     // Call the multigrid driver
00179     Vmgdriv2(iparm, rparm,
00180             &nx, &ny, &nz,
00181             u,
00182             iz, ipc, rpc,
00183             pc, ac, cc, fc,
00184             xf, yf, zf,
00185             gxcf, gycf, gzcf,
00186             alcf, a2cf, a3cf,
00187             ccf, fcf, tcf);
00188 }
00189

```

```

00190 VPUBLIC void Vmgdrv2(int *iparm, double *rparm,
00191     int *nx, int *ny, int *nz,
00192     double *u,
00193     int *iz, int *ipc, double *rpc,
00194     double *pc, double *ac, double *cc, double *fc,
00195     double *xf, double *yf, double *zf,
00196     double *gxcf, double *gycf, double *gzcf,
00197     double *alcf, double *a2cf, double *a3cf,
00198     double *ccf, double *fcf, double *tcf) {
00199
00200     // @todo Document this function
00201
00202     // Miscellaneous Variables
00203     int mgkey      = 0;
00204     int itmax      = 0;
00205     int iok        = 0;
00206     int iinfo      = 0;
00207     int istop      = 0;
00208     int ipkey      = 0;
00209     int nul        = 0;
00210     int nu2        = 0;
00211     int ilev       = 0;
00212     int ido        = 0;
00213     int iters      = 0;
00214     int ierror     = 0;
00215     int nlev_real  = 0;
00216     int ibound     = 0;
00217     int mgprol     = 0;
00218     int mgcoar     = 0;
00219     int mgsolv     = 0;
00220     int mgdisc     = 0;
00221     int mgsmoo     = 0;
00222     int iperf      = 0;
00223     int mode       = 0;
00224
00225     double epsiln  = 0.0;
00226     double epsmac  = 0.0;
00227     double errtol  = 0.0;
00228     double omegal  = 0.0;
00229     double omegan  = 0.0;
00230     double bf      = 0.0;
00231     double oh      = 0.0;
00232     double tsetupf = 0.0;
00233     double tsetupc = 0.0;
00234     double tsolve  = 0.0;
00235
00236
00237
00238     // More miscellaneous variables
00239     int itmax_p = 0;
00240     int iters_p = 0;
00241     int iok_p   = 0;
00242     int iinfo_p = 0;
00243
00244     double errtol_p = 0.0;
00245     double rho_p    = 0.0;
00246     double rho_min  = 0.0;
00247     double rho_max  = 0.0;
00248     double rho_min_mod = 0.0;
00249     double rho_max_mod = 0.0;
00250
00251     int nxf = 0;
00252     int nyf = 0;
00253     int nzf = 0;
00254     int nxc = 0;
00255     int nyc = 0;
00256     int nzc = 0;
00257     int level = 0;
00258     int nlevd = 0;
00259
00260
00261
00262     // Utility variables
00263     int numlev = 0;
00264
00265     // Get the value of nlev here because it is needed for the iz matrix
00266     int nlev = VAT(iparm, 6);
00267     MAT2(iz, 50, nlev);
00268
00269     // Decode integer parameters from the iparm array
00270     nul = VAT(iparm, 7);

```

```

00271     nu2      = VAT(iparm, 8);
00272     mgkey    = VAT(iparm, 9);
00273     itmax    = VAT(iparm, 10);
00274     istop    = VAT(iparm, 11);
00275     iinfo    = VAT(iparm, 12);
00276     ipkey    = VAT(iparm, 14);
00277     mode     = VAT(iparm, 16);
00278     mgprol   = VAT(iparm, 17);
00279     mgcoar   = VAT(iparm, 18);
00280     mgdisc   = VAT(iparm, 19);
00281     mgsmoo   = VAT(iparm, 20);
00282     mgsolv   = VAT(iparm, 21);
00283     iperf    = VAT(iparm, 22);
00284
00285     // Decode real parameters from the rparm array
00286     errtol = VAT(rparm, 1);
00287     omegal = VAT(rparm, 9);
00288     omegan = VAT(rparm, 10);
00289
00291     Vprtstp(0, -99, 0.0, 0.0, 0.0);
00292
00293     // Build the multigrid data structure in iz
00294     Vbuildstr(nx, ny, nz, &nlev, iz);
00295
00296     // Start the timer
00297     Vnm_tstart(30, "Vmgdrv2: fine problem setup");
00298
00299     // Build operator and rhs on fine grid
00300     ido = 0;
00301     Vbuildops(nx, ny, nz,
00302              &nlev, &ipkey, &iinfo, &ido, iz,
00303              &mgprol, &mgcoar, &mgsolv, &mgdisc,
00304              ipc, rpc, pc, ac, cc, fc,
00305              xf, yf, zf,
00306              gxcf, gycf, gzcf,
00307              alcf, a2cf, a3cf,
00308              ccf, fcf, tcf);
00309
00310     // Stop the timer
00311     Vnm_tstop(30, "Vmgdrv2: fine problem setup");
00312
00313     // Start the timer
00314     Vnm_tstart(30, "Vmgdrv2: coarse problem setup");
00315
00316     // Build operator and rhs on all coarse grids
00317     ido = 1;
00318     Vbuildops(nx, ny, nz,
00319              &nlev, &ipkey, &iinfo, &ido, iz,
00320              &mgprol, &mgcoar, &mgsolv, &mgdisc,
00321              ipc, rpc, pc, ac, cc, fc,
00322              xf, yf, zf,
00323              gxcf, gycf, gzcf,
00324              alcf, a2cf, a3cf,
00325              ccf, fcf, tcf);
00326
00327     // Stop the timer
00328     Vnm_tstop(30, "Vmgdrv2: coarse problem setup");
00329
00330     // Determine Machine Epsilon
00331     epsiln = Vnm_epsmac();
00332
00333     /*****
00334     *** analysis ***
00335     *** note: we destroy the rhs function "fc" here in "mpower" ***
00336     *****/
00337
00338     // errtol and itmax
00339     itmax_p = 1000;
00340     iok_p   = 0;
00341     nlev_real = nlev;
00342     nlevd    = nlev_real;
00343
00344     // Finest level initialization
00345     nxf = *nx;
00346     nyf = *ny;
00347     nzf = *nz;
00348
00349     // Go down grids: compute max/min eigenvalues of all operators
00350     for (level=1; level <= nlev_real; level++) {
00351         nlevd = nlev_real - level + 1;
00352

```



```

00353      // Move down the grids
00354      if (level != 1) {
00355
00356          // Find new grid size
00357          numlev = 1;
00358          Vmkcoors(&numlev, &nxf, &nyf, &nzf, &nxc, &nyc, &nzc);
00359
00360          // New grid size ***
00361          nxf = nxc;
00362          nyf = nyc;
00363          nzf = nzc;
00364      }
00365
00366      if (iinfo > 1) {
00367          VMESAGE3("Analysis ==> (%3d, %3d, %3d)", nxf, nyf, nzf);
00368      }
00369
00370
00371      // Largest eigenvalue of the system matrix A
00372      if (iperf == 1 || iperf == 3) {
00373
00374          if (iinfo > 1) {
00375              VMESAGE0("Power calculating rho(A)");
00376          }
00377
00378          iters_p = 0;
00379          iinfo_p = iinfo;
00380          errtol_p = 1.0e-4;
00381
00382          Vpower(&nxf, &nyf, &nzf,
00383                iz, &level,
00384                ipc, rpc, ac, cc,
00385                alcf, a2cf, a3cf, ccf,
00386                &rho_max, &rho_max_mod, &errtol_p,
00387                &itmax_p, &iters_p, &iinfo_p);
00388
00389          if (iinfo > 1) {
00390              VMESAGE1("Power iters = %d", iters_p);
00391              VMESAGE1("Power eigmax = %f", rho_max);
00392              VMESAGE1("Power (MODEL) = %f", rho_max_mod);
00393          }
00394
00395          // Smallest eigenvalue of the system matrix A
00396          if (iinfo > 1) {
00397              VMESAGE0("Ipower calculating lambda_min(A)...");
00398          }
00399
00400          iters_p = 0;
00401          iinfo_p = iinfo;
00402          errtol_p = 1.0e-4;
00403
00404          Vazeros(&nxf, &nyf, &nzf, u);
00405
00406          Vipower(&nxf, &nyf, &nzf, u, iz,
00407                alcf, a2cf, a3cf, ccf, fcf,
00408                &rho_min, &rho_min_mod, &errtol_p, &itmax_p, &iters_p,
00409                &nlevd, &level, &nlev_real, &mgsolv,
00410                &iok_p, &iinfo_p, &epsiln, &errtol, &omegal,
00411                &nul, &nu2, &mgsmo,
00412                ipc, rpc, pc, ac, cc, tcf);
00413
00414          if (iinfo > 1) {
00415              VMESAGE1("Ipower iters = %d", iters_p);
00416              VMESAGE1("Ipower eigmin = %f", rho_min);
00417              VMESAGE1("Ipower (MODEL) = %f", rho_min_mod);
00418
00419              // Condition number estimate
00420              VMESAGE1("Condition number = %f", rho_max / rho_min);
00421              VMESAGE1("Condition (MODEL) = %f", rho_max_mod / rho_min_mod);
00422          }
00423      }
00424
00425      // Spectral radius of the multigrid operator M
00426      // NOTE: due to lack of vectors, we destroy "fc" in mpower...
00427      if (iperf == 2 || iperf == 3) {
00428
00429          if (iinfo > 1) {
00430              VMESAGE0("Mpower calculating rho(M)");
00431          }
00432
00433          iters_p = 0;

```

```

00434         iinfo_p = iinfo;
00435         errtol_p = epsiln;
00436
00437         Vazeros(&nxf, &nyf, &nzf, RAT(u, VAT2(iz, 1, level)));
00438
00439         WARN_UNTESTED;
00440         Vmpower(&nxf, &nyf, &nzf, u, iz,
00441                 alcf, a2cf, a3cf, ccf, fcf,
00442                 &rho_p, &errtol_p, &itmax_p, &iters_p,
00443                 &nlevd, &level, &nlev_real, &mgsolv,
00444                 &iok_p, &iinfo_p, &epsiln,
00445                 &errtol, &omegal, &nul, &nu2, &mgs moo,
00446                 ipc, rpc, pc, ac, cc, fc, tcf);
00447
00448         if (iinfo > 1) {
00449             VMESAGE1("Mpower iters = %d", iters_p);
00450             VMESAGE1("Mpower rho(M) = %f", rho_p);
00451         }
00452     }
00453
00454     // Reinitialize the solution function
00455     Vazeros(&nxf, &nyf, &nzf, RAT(u, VAT2(iz, 1, level)));
00456
00457     // Next grid
00458 }
00459
00460 // Reinitialize the solution function
00461 Vazeros(nx, ny, nz, u);
00462
00463 /*****
00464 *** this overwrites the rhs array provided by pde specification ***
00465 **** compute an algebraically produced rhs for the given tcf ****/
00466
00467 if (istop == 4 || istop == 5 || iperf != 0) {
00468     if (iinfo > 1) {
00469         VMESAGE0("Generating algebraic RHS from your soln...");
00470     }
00471
00472     WARN_UNTESTED;
00473     Vbuidalg(nx, ny, nz, &mode, &nlev, iz,
00474             ipc, rpc, ac, cc, ccf, tcf, fc, fcf);
00475 }
00476
00477 /*****
00478 // Impose zero dirichlet boundary conditions (now in source fcn)
00479 VfboundPMG00(nx, ny, nz, u);
00480
00481 // Start the timer
00482 Vnm_tstart(30, "Vmgsdrv2: solve");
00483
00484 // Call specified multigrid method
00485 if (mode == 0 || mode == 2) {
00486     nlev_real = nlev;
00487     iok = 1;
00488     ilev = 1;
00489
00490     if (mgkey == 0) {
00491         Vmvcs(nx, ny, nz,
00492             u, iz, alcf, a2cf, a3cf, ccf,
00493             &istop, &itmax, &iters, &ierror, &nlev,
00494             &ilev, &nlev_real, &mgsolv,
00495             &iok, &iinfo, &epsiln, &errtol, &omegal,
00496             &nul, &nu2, &mgs moo,
00497             ipc, rpc, pc, ac, cc, fc, tcf);
00498     } else if (mgkey == 1) {
00499         Vmvcs(nx, ny, nz,
00500             u, iz, alcf, a2cf, a3cf, ccf,
00501             &istop, &itmax, &iters, &ierror, &nlev,
00502             &ilev, &nlev_real, &mgsolv,
00503             &iok, &iinfo, &epsiln, &errtol, &omegal,
00504             &nul, &nu2, &mgs moo,
00505             ipc, rpc, pc, ac, cc, fc, tcf);
00506     } else {
00507

```

```

00515         VABORT_MSG1("Bad mgkey given: %d", mgkey);
00516     }
00517 }
00518
00519 if (mode == 1 || mode == 2) {
00520
00521     nlev_real = nlev;
00522     iok = 1;
00523     ilev = 1;
00524
00525     if (mgkey == 0) {
00526
00527         Vmvmfas(nx, ny, nz,
00528             u, iz, alcf, a2cf, a3cf, ccf, fcf,
00529             &istop, &itmax, &iters, &ierror, &nlev,
00530             &ilev, &nlev_real, &mgsolv,
00531             &iok, &iinfo, &epsiln, &errtol, &omegan,
00532             &nul, &nu2, &mgs moo,
00533             ipc, rpc, pc, ac, cc, fc, tcf);
00534
00535     } else if (mgkey == 1) {
00536
00537         Vfmvmfas(nx, ny, nz,
00538             u, iz,
00539             alcf, a2cf, a3cf, ccf, fcf,
00540             &istop, &itmax, &iters, &ierror, &nlev,
00541             &ilev, &nlev_real, &mgsolv,
00542             &iok, &iinfo, &epsiln, &errtol, &omegan,
00543             &nul, &nu2, &mgs moo,
00544             ipc, rpc, pc, ac, cc, fc, tcf);
00545
00546     } else {
00547         VABORT_MSG1("Bad mgkey given: %d", mgkey);
00548     }
00549 }
00550
00551 // Stop the timer
00552 Vnm_tstop(30, "Vmgsdrv2: solve");
00553
00554 // Restore boundary conditions
00555 ibound = 1;
00556
00557 VfboundPMG(&ibound, nx, ny, nz, u, gxcf, gycf, gzcf);
00558 }
00559
00560
00561
00562 VPUBLIC void Vmgsz(int *mgcoar, int *mgdisc, int *mgsolv,
00563     int *nx, int *ny, int *nz,
00564     int *nlev,
00565     int *nxc, int *nyc, int *nzc,
00566     int *nf, int *nc,
00567     int *narr, int *narrc,
00568     int *n_rpc, int *n_iz, int *n_ipc,
00569     int *iretot, int *iintot) {
00570
00571     // Constants: num of different types of arrays in mg code
00572     int num_nf = 0;
00573     int num_narr = 2;
00574     int num_narrc = 27;
00575
00576     // Misc variables
00577     int nc_band, num_band, n_band;
00578     int nxf, nyf, nzf;
00579     int level;
00580     int num_nf_oper, num_narrc_oper;
00581
00582     // Utility variables
00583     int numlev;
00584
00585     // Go down grids: compute max/min eigenvalues of all operators
00586     *nf = *nx * *ny * *nz;
00587
00588     *narr = *nf;
00589
00590     nxf = *nx;
00591     nyf = *ny;
00592     nzf = *nz;
00593
00594     *nxc = *nx;
00595     *nyc = *ny;

```

```

00596     *nzc = *nz;
00597
00598     for (level=2; level<=*nlev; level++) {
00599
00600         //find new grid size ***
00601
00602         numlev = 1;
00603         Vmkcors(&numlev, &nxf, &nyf, &nzf, nxc, nyc, nzc);
00604
00605         // New grid size
00606         nxf = *nxc;
00607         nyf = *nyc;
00608         nzf = *nzc;
00609
00610         // Add the unknowns on this level to the total
00611         *narr += nxf * nyf * nzf;
00612     }
00613     *nc = *nxc * *nyc * *nzc;
00614     *narrc = *narr - *nf;
00615
00616     // Box or fem on fine grid?
00617     if (*mgdisc == 0) {
00618         num_nf_oper = 4;
00619     } else if (*mgdisc == 1) {
00620         num_nf_oper = 14;
00621     } else {
00622         Vnm_print(2, "Vmgsz: invalid mgdisc parameter: %d\n", *mgdisc);
00623     }
00624
00625     // Galerkin or standard coarsening?
00626     if ((*mgcoar == 0 || *mgcoar == 1) && *mgdisc == 0) {
00627         num_narrc_oper = 4;
00628     } else if (*mgcoar == 2) {
00629         num_narrc_oper = 14;
00630     } else {
00631         Vnm_print(2, "Vmgsz: invalid mgcoar parameter: %d\n", *mgcoar);
00632     }
00633
00634     // Symmetric banded linpack storage on coarse grid
00635     if (*mgsolv == 0) {
00636         n_band = 0;
00637     } else if (*mgsolv == 1) {
00638         if ((*mgcoar == 0 || *mgcoar == 1) && *mgdisc == 0) {
00639             num_band = 1 + (*nxc - 2) * (*nyc - 2);
00640         } else {
00641             num_band = 1 + (*nxc - 2) * (*nyc - 2) + (*nxc - 2) + 1;
00642         }
00643         nc_band = (*nxc - 2) * (*nyc - 2) * (*nzc - 2);
00644         n_band = nc_band * num_band;
00645     } else {
00646         Vnm_print(2, "Vmgsz: invalid mgsolv parameter: %d\n", *mgsolv);
00647     }
00648
00649     // Info work array required storage
00650     *n_rpc = 100 * (*nlev + 1);
00651
00652     // Resulting total required real storage for method
00653     *iretot = num_narr * *narr
00654             + (num_nf + num_nf_oper) * *nf
00655             + (num_narrc + num_narrc_oper) * *narrc
00656             + n_band
00657             + *n_rpc;
00658
00659     // The integer storage parameters ***
00660     *n_iz = 50 * (*nlev + 1);
00661     *n_ipc = 100 * (*nlev + 1);
00662
00663     // Resulting total required integer storage for method
00664     *iintot = *n_iz + *n_ipc;
00665 }

```

9.131 mgdrvd.h

```

00001
00054 #ifndef _MGDRVD_H_
00055 #define _MGDRVD_H_
00056
00057 #include "apbscfg.h"

```

```
00058
00059 #include "malloc/malloc.h"
00060
00061 #include "generic/vhal.h"
00062 #include "generic/vmatrix.h"
00063 #include "pmgc/mgsabd.h"
00064 #include "pmgc/mgcsd.h"
00065 #include "pmgc/powerd.h"
00066 #include "pmgc/mgfasd.h"
00067
00074 VEXTERNC void Vmgdriv(
00075     int* iparm,
00076     double* rparm,
00077     int* iwork,
00078     double* rwork,
00079     double* u,
00080     double* xf,
00081     double* yf,
00082     double* zf,
00083     double* gxcf,
00084     double* gycf,
00085     double* gzcf,
00086     double* alcf,
00087     double* a2cf,
00088     double* a3cf,
00089     double* ccf,
00090     double* fcf,
00091     double* tcf
00092 );
00093
00130 VEXTERNC void Vmgdriv2(
00131     int *iparm,
00132     double *rparm,
00133     int *nx,
00134     int *ny,
00135     int *nz,
00136     double *u,
00137     int *iz,
00138     int *ipc,
00139     double *rpc,
00140     double *pc,
00141     double *ac,
00142     double *cc,
00143     double *fc,
00144     double *xf,
00145     double *yf,
00146     double *zf,
00147     double *gxcf,
00148     double *gycf,
00149     double *gzcf,
00150     double *alcf,
00151     double *a2cf,
00152     double *a3cf,
00153     double *ccf,
00154     double *fcf,
00155     double *tcf
00156 );
00157
00158
00159
00229 VEXTERNC void Vmgsz(
00230     int *mgcoar,
00231     int *mgdisc,
00232     int *mgsolv,
00233     int *nx,
00234     int *ny,
00235     int *nz,
00236     int *nlev,
00237     int *nxc,
00238     int *nyc,
00239     int *nzc,
00240     int *nf,
00241     int *nc,
00242     int *narr,
00243     int *narrc,
00244     int *n_rpc,
00245     int *n_iz,
00246     int *n_ipc,
00247     int *iretot,
00248     int *iintot
00249 );
```

```

00250
00251
00252
00253 #endif /* _MGDRVD_H_ */

```

9.132 mgfasd.c

```

00001
00055 #include "mgfasd.h"
00056
00057 VPUBLIC void Vfmvfas(int *nx, int *ny, int *nz,
00058     double *x,
00059     int *iz,
00060     double *w0, double *w1, double *w2, double *w3, double *w4,
00061     int *istop, int *itmx, int *iters, int *ierror,
00062     int *nlev, int *ilev, int *nlev_real,
00063     int *mgsolv, int *iok, int *iinfo,
00064     double *epsiln, double *errtol, double *omega,
00065     int *nul, int *nu2, int *mgsmoo,
00066     int *ipc, double *rpc,
00067     double *pc, double *ac, double *cc, double *fc, double *tru) {
00068
00069     // Other Declarations
00070     int level, itmx, nlevd, iterd, iokd;
00071     int nxf, nyf, nzf;
00072     int nxc, nyc, nzc;
00073     int istpd, iinfod;
00074     double errd;
00075
00076     // Utility variables
00077     int numlev;
00078
00079     MAT2(iz, 50, *nlev);
00080
00081     // Recover gridsizes
00082     nxf = *nx;
00083     nyf = *ny;
00084     nzf = *nz;
00085
00086     numlev = *nlev - 1;
00087     Vmkcors(&numlev, &nxf, &nyf, &nzf, &nxc, &nyc, &nzc);
00088
00089     // Move up grids: interpolate solution to finer, do v cycle
00090     if (*iinfo != 0) {
00091
00092         Vnm_print(2, "Vfmvfas: starting: (%d,%d,%d) (%d,%d,%d)\n",
00093             nxf, nyf, nzf, nxc, nyc, nzc);
00094     }
00095
00096     for (level = *nlev_real; level >= *ilev + 1; level--) {
00097
00098         // Call mv cycle
00099         errd = 1.0e-5;
00100         itmx = 1;
00101         nlevd = *nlev_real - level + 1;
00102         iterd = 0;
00103         iokd = 2;
00104         iinfod = *iinfo;
00105         istpd = *istop;
00106         if (*iinfo >= 2)
00107             iokd = 2;
00108
00109         Vmvfas(&nxc, &nyc, &nzc,
00110             x,
00111             iz,
00112             w0, w1, w2, w3, w4,
00113             &istpd, &itmx, &iterd, ierror,
00114             &nlevd, &level, nlev_real,
00115             mgsolv, &iokd, &iinfod,
00116             epsiln, errtol, omega,
00117             nul, nu2, mgsmoo,
00118             ipc, rpc,
00119             pc, ac, cc, fc, tru);
00120
00121         // Find new grid size
00122         numlev = 1;
00123         Vmkfine(&numlev, &nxc, &nyc, &nzc, &nxf, &nyf, &nzf);
00124

```

```

00125         // Interpolate to next finer grid
00126         VinterpPMG(&nxc, &nyc, &nzc,
00127                   &nxf, &nyf, &nzf,
00128                   RAT( x, VAT2(iz, 1, level)),
00129                   RAT( x, VAT2(iz, 1, level-1)),
00130                   RAT(pc, VAT2(iz, 11, level-1)));
00131
00132         // New grid size
00133         nxc = nxf;
00134         nyc = nyf;
00135         nzc = nzf;
00136     }
00137
00138
00139
00140     // Call mv cycle
00141     level = *ilev;
00142
00143     Vmvfas(&nxf, &nyf, &nzf,
00144           x, iz,
00145           w0, w1, w2, w3, w4,
00146           istop, itmax, iters,
00147           ierror, nlev, &nlev_real,
00148           mgsolv, iok, iinfo,
00149           epsiln, errtol, omega,
00150           nul, nu2, mgsmoo,
00151           ipc, rpc,
00152           pc, ac, cc, fc, tru);
00153 }
00154
00155
00156
00157 VPUBLIC void Vmvfas(int *nx, int *ny, int *nz,
00158                   double *x,
00159                   int *iz,
00160                   double *w0, double *w1, double *w2, double *w3, double *w4,
00161                   int *istop, int *itmax, int *iters, int *ierror,
00162                   int *nlev, int *ilev, int *nlev_real,
00163                   int *mgsolv, int *iok, int *iinfo,
00164                   double *epsiln, double *errtol, double *omega,
00165                   int *nul, int *nu2, int *mgsmoo,
00166                   int *ipc, double *rpc,
00167                   double *pc, double *ac, double *cc, double *fc, double *tru) {
00168
00169     // Other declarations
00170     int level, lev;
00171     int itmax_s, iters_s, nuuu, ivariv, mgsmoo_s, iresid;
00172     int nxf, nyf, nzf;
00173     int nxc, nyc, nzc;
00174     int iadjoint;
00175     double errtol_s;
00176     double rsden, rsnm, orsnrm;
00177     double xdamp;
00178
00179     int numlev;
00180     double alpha;
00181
00182     MAT2(iz, 50, *nlev);
00183
00184     WARN_UNTESTED;
00185
00186     // Recover level information
00187     level = 1;
00188     lev = (*ilev - 1) + level;
00189
00190     // Recover gridsizes
00191     nxf = *nx;
00192     nyf = *ny;
00193     nzf = *nz;
00194
00195     numlev = *nlev - 1;
00196     Vmkcors(&numlev, &nxf, &nyf, &nzf, &nxc, &nyc, &nzc);
00197
00198     // Do some i/o if requested
00199     if (*iinfo != 0) {
00200         Vnm_print(2, "Vmvfas: starting: (%d, %d, %d) (%d, %d, %d)\n",
00201                 nxf, nyf, nzf, nxc, nyc, nzc);
00202     }
00203
00204     // Initial wall clock
00205     if (*iok != 0) {

```

```

00206     Vprtstp(*iok, -1, 0.0, 0.0, 0.0);
00207 }
00208
00209 /*****
00210 *** note: if (iok != 0) then: use a stopping test. ***
00211 *** else: use just the itmax to stop iteration. ***
00212 *****/
00213 *** istop=0 most efficient (whatever it is) ***
00214 *** istop=1 relative residual ***
00215 *** istop=2 rms difference of successive iterates ***
00216 *** istop=3 relative true error (provided for testing) ***
00217 *****/
00218
00219 // Compute denominator for stopping criterion
00220 if (*iok != 0) {
00221     if (*istop == 0) {
00222         rsden = 1.0;
00223     } else if (*istop == 1) {
00224
00225         // Compute initial residual with zero initial guess
00226         // this is analogous to the linear case where one can
00227         // simply take norm of rhs for a zero initial guess
00228         Vazeros(&nxf, &nyf, &nzf, w1);
00229
00230         Vnmresid(&nxf, &nyf, &nzf,
00231                 RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00232                 RAT(ac, VAT2(iz, 7, lev)), RAT(cc, VAT2(iz, 1, lev)),
00233                 RAT(fc, VAT2(iz, 1, lev)),
00234                 w1, w2, w3);
00235
00236         rsden = Vxnrm1(&nxf, &nyf, &nzf, w2);
00237
00238     } else if (*istop == 2) {
00239         rsden = VSQRT(nxf * nyf * nzf);
00240     } else if (*istop == 3) {
00241         rsden = Vxnrm2(&nxf, &nyf, &nzf, RAT(tru, VAT2(iz, 1, lev)));
00242     } else if (*istop == 4) {
00243         rsden = Vxnrm2(&nxf, &nyf, &nzf, RAT(tru, VAT2(iz, 1, lev)));
00244     } else if (*istop == 5) {
00245         Vnmvec(&nxf, &nyf, &nzf,
00246               RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00247               RAT(ac, VAT2(iz, 7, lev)), RAT(cc, VAT2(iz, 1, lev)),
00248               RAT(tru, VAT2(iz, 1, lev)),
00249               w1, w2);
00250         rsden = VSQRT(Vxdot(&nxf, &nyf, &nzf, RAT(tru, VAT2(iz, 1, lev)), w1));
00251     } else {
00252         Vnm_print(2, "Vmfas: bad istop value: %d\n", *istop);
00253     }
00254     if (rsden == 0.0) {
00255         rsden = 1.0;
00256         Vnm_print(2, "Vmfas: rhs is zero on finest level\n");
00257     }
00258     rsnm = rsden;
00259     orsnrm = rsnm;
00260
00261     Vprtstp(*iok, 0, rsnm, rsden, orsnrm);
00262 }
00263
00264
00265 /*****
00266 *** solve directly if nlev = 1
00267 *****/
00268
00269 // Solve directly if on the coarse grid
00270 if (*nlev == 1) {
00271
00272     //solve with ncghs, mgsmoo_s=4 (no residual)
00273     iresid = 0;
00274     iadjoint = 0;
00275     itmax_s = 100;
00276     iters_s = 0;
00277     errtol_s = *epsiln;
00278     mgsmoo_s = *mgsmoo;
00279     Vazeros(&nxf, &nyf, &nzf, RAT(x, VAT2(iz, 1, lev)));
00280     Vnsmooth(&nxf, &nyf, &nzf,
00281             RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00282             RAT(ac, VAT2(iz, 7, lev)), RAT(cc, VAT2(iz, 1, lev)),
00283             RAT(fc, VAT2(iz, 1, lev)),
00284             RAT(x, VAT2(iz, 1, lev)),
00285             w1, w2, w3,

```



```

00287         &itmax_s, &iters_s, &errtol_s, omega,
00288         &iresid, &iadjoin, &mgsmoo_s);
00289
00290     // Compute the stopping test
00291     *iters = 1;
00292     if (*iok != 0) {
00293         orsnrm = rsnm;
00294         if (*istop == 0) {
00295             Vnmresid(&nxf, &nyf, &nzf,
00296                     RAT(ipc, VAT2(iz, 5, lev)),
00297                     RAT(rpc, VAT2(iz, 6, lev)),
00298                     RAT(ac, VAT2(iz, 7, lev)),
00299                     RAT(cc, VAT2(iz, 1, lev)),
00300                     RAT(fc, VAT2(iz, 1, lev)),
00301                     RAT(x, VAT2(iz, 1, lev)),
00302                     w1, w2);
00303             rsnm = Vxnrm1(&nxf, &nyf, &nzf, w1);
00304         } else if (*istop == 1) {
00305             Vnmresid(&nxf, &nyf, &nzf,
00306                     RAT(ipc, VAT2(iz, 5, lev)),
00307                     RAT(rpc, VAT2(iz, 6, lev)),
00308                     RAT(ac, VAT2(iz, 7, lev)),
00309                     RAT(cc, VAT2(iz, 1, lev)),
00310                     RAT(fc, VAT2(iz, 1, lev)),
00311                     RAT(x, VAT2(iz, 1, lev)),
00312                     w1, w2);
00313             rsnm = Vxnrm1(&nxf, &nyf, &nzf, w1);
00314         } else if (*istop == 2) {
00315             Vxcopy(&nxf, &nyf, &nzf,
00316                  RAT(tru, VAT2(iz, 1, lev)),
00317                  w1);
00318             alpha = -1.0;
00319             Vxaxpy(&nxf, &nyf, &nzf,
00320                   &alpha, RAT(x, VAT2(iz, 1, lev)), w1);
00321             rsnm = Vxnrm1(&nxf, &nyf, &nzf, w1);
00322             Vxcopy(&nxf, &nyf, &nzf,
00323                   RAT(x, VAT2(iz, 1, lev)),
00324                   RAT(tru, VAT2(iz, 1, lev)));
00325         } else if (*istop == 3) {
00326             Vxcopy(&nxf, &nyf, &nzf,
00327                  RAT(tru, VAT2(iz, 1, lev)),
00328                  w1);
00329             alpha = -1.0;
00330             Vxaxpy(&nxf, &nyf, &nzf,
00331                   &alpha, RAT(x, VAT2(iz, 1, lev)), w1);
00332             rsnm = Vxnrm2(&nxf, &nyf, &nzf, w1);
00333         } else if (*istop == 4) {
00334             Vxcopy(&nxf, &nyf, &nzf,
00335                  RAT(tru, VAT2(iz, 1, lev)),
00336                  w1);
00337             alpha = -1.0;
00338             Vxaxpy(&nxf, &nyf, &nzf,
00339                   &alpha, RAT(x, VAT2(iz, 1, lev)), w1);
00340             rsnm = Vxnrm2(&nxf, &nyf, &nzf, w1);
00341         } else if (*istop == 5) {
00342             Vxcopy(&nxf, &nyf, &nzf,
00343                  RAT(tru, VAT2(iz, 1, lev)),
00344                  w1);
00345             alpha = -1.0;
00346             Vxaxpy(&nxf, &nyf, &nzf,
00347                   &alpha, RAT(x, VAT2(iz, 1, lev)), w1);
00348             Vnmatvec(&nxf, &nyf, &nzf,
00349                    RAT(ipc, VAT2(iz, 5, lev)),
00350                    RAT(rpc, VAT2(iz, 6, lev)),
00351                    RAT(ac, VAT2(iz, 7, lev)),
00352                    RAT(cc, VAT2(iz, 1, lev)),
00353                    w1, w2, w3);
00354             rsnm = VSQRT(Vxdot(&nxf, &nyf, &nzf, w1, w2));
00355         } else {
00356             Vnm_print(2, "Vmvcs: bad istop value: %d\n", *istop);
00357         }
00358
00359         Vprtstp(*iok, *iters, rsnm, rsden, orsnrm);
00360     }
00361     return;
00362 }
00363
00364 /*****
00365 *** begin mg iteration (note nxf,nyf,nzf changes during loop)
00366 *****/
00367

```

```

00368 // setup for the v-cycle looping ***
00369 *iters = 0;
00370 while(1) {
00371
00372     // Finest level initialization
00373     level = 1;
00374     lev = (*ilev - 1) + level;
00375
00376     // Nul pre-smoothings on fine grid (with residual)
00377     iresid = 1;
00378     iadjoint = 0;
00379     iters_s = 0;
00380     errtol_s = 0.0;
00381     nuuu = Vivariv(nul, &lev);
00382     Vnsmooth(&nxf, &nyf, &nzf,
00383             RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00384             RAT(ac, VAT2(iz, 7, lev)), RAT(cc, VAT2(iz, 1, lev)),
00385             RAT(fc, VAT2(iz, 1, lev)), RAT(x, VAT2(iz, 1, lev)),
00386             w2, w3, w1,
00387             &nuuu, &iters_s, &errtol_s, omega,
00388             &iresid, &iadjoint, mgsmoo);
00389     Vxcopy(&nxf, &nyf, &nzf, w1, RAT(w0, VAT2(iz, 1, lev)));
00390
00391     /* *****
00392     * begin cycling down to coarse grid
00393     * *****/
00394
00395     // Go down grids: restrict resid to coarser and smooth
00396     for (level = 2; level <= *nlev; level++) {
00397         lev = (*ilev - 1) + level;
00398
00399         // Find new grid size
00400         numlev = 1;
00401         Vmkcors(&numlev, &nxf, &nyf, &nzf, &nxc, &nyc, &nzc);
00402
00403         // Restrict residual to coarser grid
00404         Vrestrc(&nxf, &nyf, &nzf, &nxc, &nyc, &nzc,
00405               w1, RAT(w0, VAT2(iz, 1, lev)),
00406               RAT(pc, VAT2(iz, 11, lev-1)));
00407
00408         // Restrict (extract) solution to coarser grid
00409         Vextrac(&nxf, &nyf, &nzf, &nxc, &nyc, &nzc,
00410               RAT(x, VAT2(iz, 1, lev-1)), RAT(w4, VAT2(iz, 1, lev)));
00411
00412         // New grid size
00413         nxf = nxc;
00414         nyf = nyc;
00415         nzf = nzc;
00416
00417         // Apply coarse grid operator to coarse grid soln
00418         Vnmatvec(&nxf, &nyf, &nzf,
00419               RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00420               RAT(ac, VAT2(iz, 7, lev)), RAT(cc, VAT2(iz, 1, lev)),
00421               RAT(w4, VAT2(iz, 1, lev)), RAT(fc, VAT2(iz, 1, lev)),
00422               w3);
00423
00424         // Build coarse grid right hand side
00425         alpha = 1.0;
00426         Vxaxpy(&nxf, &nyf, &nzf, &alpha,
00427               RAT(w0, VAT2(iz, 1, lev)), RAT(fc, VAT2(iz, 1, lev)));
00428
00429         // If not on coarsest level yet...
00430         if (level != *nlev) {
00431
00432             // nul pre-smoothings on this level (with residual)
00433             Vxcopy(&nxf, &nyf, &nzf,
00434                   RAT(w4, VAT2(iz, 1, lev)), RAT(x, VAT2(iz, 1, lev)));
00435             iresid = 1;
00436             iadjoint = 0;
00437             iters_s = 0;
00438             errtol_s = 0.0;
00439             nuuu = Vivariv(nul, &lev);
00440             Vnsmooth(&nxf, &nyf, &nzf,
00441                   RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00442                   RAT(ac, VAT2(iz, 7, lev)), RAT(cc, VAT2(iz, 1, lev)),
00443                   RAT(fc, VAT2(iz, 1, lev)),
00444                   RAT(x, VAT2(iz, 1, lev)),
00445                   w2, w3, w1,
00446                   &nuuu, &iters_s, &errtol_s, omega,
00447                   &iresid, &iadjoint, mgsmoo);
00448         }

```

```

00449
00450 // End of cycling down to coarse grid loop
00451 }
00452
00453
00454
00455 /* *****
00456 * begin coarse grid
00457 * *****/
00458
00459 // Coarsest level
00460 level = *nlev;
00461 lev = (*ilev - 1) + level;
00462
00463 // Solve on coarsest grid with ncghs, mgsmoo_s=4 (no residual)
00464 iresid = 0;
00465 iadjoint = 0;
00466 itmax_s = 100;
00467 iters_s = 0;
00468 errtol_s = *epsiln;
00469 mgsmoo_s = *mgsmoo;
00470 Vazeros(&nxf, &nyf, &nzf, RAT(x, VAT2(iz, 1, lev)));
00471 Vnsmooth(&nxf, &nyf, &nzf,
00472          RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00473          RAT(ac, VAT2(iz, 7, lev)), RAT(cc, VAT2(iz, 1, lev)),
00474          RAT(fc, VAT2(iz, 1, lev)),
00475          RAT(x, VAT2(iz, 1, lev)),
00476          w1, w2, w3,
00477          &itmax_s, &iters_s, &errtol_s, omega,
00478          &iresid, &iadjoint, &mgsmoo_s);
00479
00480 /* *****
00481 * begin cycling back to fine grid
00482 * *****/
00483
00484 // Move up grids: interpolate resid to finer and smooth
00485 for (level = *nlev - 1; level >= 1; level--) {
00486     lev = (*ilev - 1) + level;
00487
00488     // Find new grid size
00489     numlev = 1;
00490     Vmkfine(&numlev, &nxf, &nyf, &nzf, &nxc, &nyc, &nzc);
00491
00492     // Form difference of new approx at the coarse grid
00493     alpha = -1.0;
00494     Vxaxy(&nxf, &nyf, &nzf, &alpha,
00495          RAT(w4, VAT2(iz, 1, lev + 1)), RAT(x, VAT2(iz, 1, lev + 1)));
00496
00497     // Call the line search (on the coarser level)
00498     Vlinesearch(&nxf, &nyf, &nzf, &xdamp,
00499                RAT(ipc, VAT2(iz, 5, lev + 1)),
00500                RAT(rpc, VAT2(iz, 6, lev + 1)),
00501                RAT(ac, VAT2(iz, 7, lev + 1)),
00502                RAT(cc, VAT2(iz, 1, lev + 1)),
00503                RAT(fc, VAT2(iz, 1, lev + 1)),
00504                RAT(x, VAT2(iz, 1, lev + 1)),
00505                RAT(w4, VAT2(iz, 1, lev + 1)),
00506                RAT(w0, VAT2(iz, 1, lev + 1)),
00507                w1, w2, w3);
00508
00509     // Interpolate to next finer grid
00510     VinterpPMG(&nxf, &nyf, &nzf, &nxc, &nyc, &nzc,
00511               RAT(x, VAT2(iz, 1, lev + 1)),
00512               w1,
00513               RAT(pc, VAT2(iz, 11, lev)));
00514
00515     // New grid size
00516     nxf = nxc;
00517     nyf = nyc;
00518     nzf = nzc;
00519
00520     // Perform the coarse grid correction
00521     Vxaxy(&nxf, &nyf, &nzf, &xdamp, w1, RAT(x, VAT2(iz, 1, lev)));
00522
00523     // nu2 post-smoothings for correction (no residual) ***
00524     iresid = 0;
00525     iadjoint = 1;
00526     iters_s = 0;
00527     errtol_s = 0.0;
00528     nuuu = Vivariv(nu2, &lev);
00529     Vnsmooth(&nxf, &nyf, &nzf,

```

```

00530         RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00531         RAT( ac, VAT2(iz, 7, lev)), RAT( cc, VAT2(iz, 1, lev)),
00532         RAT( fc, VAT2(iz, 1, lev)),
00533         RAT( x, VAT2(iz, 1, lev)),
00534         w1, w2, w3,
00535         &nuuu, &iters_s, &errtol_s, omega,
00536         &iresid, &iadjoint, mgsmoo);
00537     }
00538
00539
00540
00541     /* *****
00542     * iteration complete: do some i/o
00543     * ***** */
00544
00545     // Increment the iteration counter
00546     iters = iters + 1;
00547
00548     // Compute/check the current stopping test
00549     if (*iok != 0) {
00550         orsnrm = rsnm;
00551         if (*istop == 0) {
00552             Vnmresid(&nxf, &nyf, &nzf,
00553                 RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00554                 RAT( ac, VAT2(iz, 7, lev)), RAT( cc, VAT2(iz, 1, lev)),
00555                 RAT( fc, VAT2(iz, 1, lev)), RAT( x, VAT2(iz, 1, lev)),
00556                 w1, w2);
00557             rsnm = Vxnrm1(&nxf, &nyf, &nzf, w1);
00558         } else if (*istop == 1) {
00559             Vnmresid(&nxf, &nyf, &nzf,
00560                 RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00561                 RAT( ac, VAT2(iz, 7, lev)), RAT( cc, VAT2(iz, 1, lev)),
00562                 RAT( fc, VAT2(iz, 1, lev)), RAT( x, VAT2(iz, 1, lev)),
00563                 w1, w2);
00564             rsnm = Vxnrm1(&nxf, &nyf, &nzf, w1);
00565         } else if (*istop == 2) {
00566             Vxcopy(&nxf, &nyf, &nzf, RAT(tru, VAT2(iz, 1, lev)), w1);
00567             alpha = -1.0;
00568             Vxaxpy(&nxf, &nyf, &nzf, &alpha, RAT(x, VAT2(iz, 1, lev)), w1);
00569             rsnm = Vxnrm1(&nxf, &nyf, &nzf, w1);
00570             Vxcopy(&nxf, &nyf, &nzf,
00571                 RAT( x, VAT2(iz, 1, lev)),
00572                 RAT(tru, VAT2(iz, 1, lev)));
00573         } else if (*istop == 3) {
00574             Vxcopy(&nxf, &nyf, &nzf, RAT(tru, VAT2(iz, 1, lev)), w1);
00575             alpha = -1.0;
00576             Vxaxpy(&nxf, &nyf, &nzf, &alpha, RAT(x, VAT2(iz, 1, lev)), w1);
00577             rsnm = Vxnrm2(&nxf, &nyf, &nzf, w1);
00578         } else if (*istop == 4) {
00579             Vxcopy(&nxf, &nyf, &nzf, RAT(tru, VAT2(iz, 1, lev)), w1);
00580             alpha = -1.0;
00581             Vxaxpy(&nxf, &nyf, &nzf, &alpha, RAT(x, VAT2(iz, 1, lev)), w1);
00582             rsnm = Vxnrm2(&nxf, &nyf, &nzf, w1);
00583         } else if (*istop == 5) {
00584             Vxcopy(&nxf, &nyf, &nzf, RAT(tru, VAT2(iz, 1, lev)), w1);
00585             alpha = -1.0;
00586             Vxaxpy(&nxf, &nyf, &nzf, &alpha, RAT(x, VAT2(iz, 1, lev)), w1);
00587             Vnmatvec(&nxf, &nyf, &nzf,
00588                 RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00589                 RAT( ac, VAT2(iz, 7, lev)), RAT( cc, VAT2(iz, 1, lev)),
00590                 w1, w2, w3);
00591             rsnm = VSQRT(Vxdot(&nxf, &nyf, &nzf, w1, w2));
00592         } else {
00593             VABORT_MSG1("Bad istop value: %d", *istop);
00594         }
00595         Vprtstp(*iok, *iters, rsnm, rsden, orsnrm);
00596
00597         if ((rsnm / rsden) <= *errtol)
00598             break;
00599     }
00600
00601     if (*iters >= *itmax) {
00602         *ierror = 1;
00603         break;
00604     }
00605 }
00606 }

```

9.133 mgfasd.h

```
00001
00049 #ifndef _MGFASD_H_
00050 #define _MGFASD_H_
00051
00052 #include "apbscfg.h"
00053
00054 #include "malloc/malloc.h"
00055
00056 #include "generic/vhal.h"
00057 #include "pmgc/smoothd.h"
00058 #include "pmgc/mgsudd.h"
00059
00072 VEXTERNC void Vfmvfas(
00073     int      *nx,
00074     int      *ny,
00075     int      *nz,
00076     double   *x,
00077     int      *iz,
00078     double   *w0,
00079     double   *w1,
00080     double   *w2,
00081     double   *w3,
00082     double   *w4,
00083     int      *istop,
00084     int      *itmax,
00085     int      *iters,
00086     int      *ierror,
00087     int      *nlev,
00088     int      * ilev,
00089     int      *nlev_real,
00090     int      *mgsolv,
00091     int      *iok,
00092     int      *iinfo,
00093     double   *epsiln,
00094     double   *errtol,
00095     double   *omega,
00096     int      *nul,
00097     int      *nu2,
00098     int      *mgsmoo,
00099     int      *ipc,
00100     double   *rpc,
00101     double   *pc,
00102     double   *ac,
00103     double   *cc,
00104     double   *fc,
00105     double   *tru
00106 );
00107
00108
00109
00151 VEXTERNC void Vmvfas(
00152     int      *nx,
00153     int      *ny,
00154     int      *nz,
00155     double   *x,
00156     int      *iz,
00157     double   *w0,
00158     double   *w1,
00159     double   *w2,
00160     double   *w3,
00161     double   *w4,
00162     int      *istop,
00163     int      *itmax,
00164     int      *iters,
00165     int      *ierror,
00166     int      *nlev,
00167     int      *ilev,
00168     int      *nlev_real,
00169     int      *mgsolv,
00170     int      *iok,
00171     int      *iinfo,
00172     double   *epsiln,
00173     double   *errtol,
00174     double   *omega,
00175     int      *nul,
00176     int      *nu2,
00177     int      *mgsmoo,
00178     int      *ipc,
```

```

00179         double      *rpc,
00180         double      *pc,
00181         double      *ac,
00182         double      *cc,
00183         double      *fc,
00184         double      *tru
00185     );
00186
00187 #endif /* _MGFASD_H_ */
00188

```

9.134 mgsbdc.c

```

00001
00055 #include "mgsbdc.h"
00056
00057 VPUBLIC void Vbuildops(
00058     int *nx, int *ny, int *nz,
00059     int *nlev, int *ipkey, int *iinfo,
00060     int *ido, int *iz,
00061     int *mgprol, int *mgcoar, int *mgsolv, int *mgdisc, int *ipc,
00062     double *rpc, double *pc, double *ac, double *cc, double *fc,
00063     double *xf, double *yf, double *zf,
00064     double *gxcf, double *gycf, double *gzcf,
00065     double *alcf, double *a2cf, double *a3cf,
00066     double *ccf, double *fcf, double *tcf
00067 ) {
00068
00069     // @todo Document this function
00070     int lev = 0;
00071     int nxx = 0;
00072     int nyy = 0;
00073     int nzz = 0;
00074     int nxold = 0;
00075     int nyold = 0;
00076     int nzold = 0;
00077     int numdia = 0;
00078     int key = 0;
00079
00080     // Utility variables
00081     int i;
00082
00083     MAT2(iz, 50, *nlev);
00084
00085     // Setup
00086     nxx = *nx;
00087     nyy = *ny;
00088     nzz = *nz;
00089
00090     // Build the operator a on the finest level
00091     if (*ido == 0 || *ido == 2) {
00092
00093         lev = 1;
00094
00095         // Some i/o
00096         if (*iinfo > 0)
00097             VMESSAGE3("Fine: (%03d, %03d, %03d)", nxx, nyy, nzz);
00098
00099         // Finest level discretization
00100         VbuildA(&nxx, &nyy, &nzz,
00101             ipkey, mgdisc, &numdia,
00102             RAT(ipc, VAT2(iz, 5,lev)), RAT(rpc, VAT2(iz, 6,lev)),
00103             RAT(ac, VAT2(iz, 7,lev)), RAT(cc, VAT2(iz, 1,lev)), RAT(fc, VAT2(iz, 1,lev)),
00104             RAT(xf, VAT2(iz, 8,lev)), RAT(yf, VAT2(iz, 9,lev)), RAT(zf, VAT2(iz, 10,lev)),
00105             RAT(gxcf, VAT2(iz, 2,lev)), RAT(gycf, VAT2(iz, 3,lev)), RAT(gzcf, VAT2(iz, 4,lev)),
00106             RAT(alcf, VAT2(iz, 1,lev)), RAT(a2cf, VAT2(iz, 1,lev)), RAT(a3cf, VAT2(iz, 1,lev)),
00107             RAT(ccf, VAT2(iz, 1,lev)), RAT(fcf, VAT2(iz, 1,lev)));
00108
00109         VMESSAGE2("Operator stencil (lev, numdia) = (%d, %d)", lev, numdia);
00110
00111         // Now initialize the differential operator offset
00112         VAT2(iz, 7, lev+1) = VAT2(iz, 7, lev) + numdia * nxx * nyy * nzz;
00113
00114         // Debug
00115         if (*iinfo > 7) {
00116             Vprtmatd(&nxx, &nyy, &nzz,
00117                 RAT(ipc, VAT2(iz, 5,lev)), RAT(rpc, VAT2(iz, 6,lev)), RAT(ac, VAT2(iz, 7,lev)));
00118         }
00119     }
00120

```

```

00119     }
00120
00121     // Build the (nlev-1) level operators
00122     if (*ido == 1 || *ido == 2 || *ido == 3) {
00123
00124         for (lev=2; lev<=*nlev; lev++) {
00125             nxold = nxx;
00126             nyold = nyy;
00127             nzold = nzz;
00128             i = 1;
00129
00130
00131             Vmkcors(&i, &nxold, &nyold, &nzold, &nxx, &nyy, &nzz);
00132             if (*ido != 3) {
00133
00134                 // Build the interpolation operator on this level
00135                 VbuildP(&nxold, &nyold, &nzold,
00136                     &nxx, &nyy, &nzz,
00137                     mgprol,
00138                     RAT(ipc, VAT2(iz, 5,lev-1)), RAT(rpc, VAT2(iz, 6,lev-1)),
00139                     RAT(pc, VAT2(iz, 11,lev-1)), RAT(ac, VAT2(iz, 7,lev-1)),
00140                     RAT(xf, VAT2(iz, 8,lev-1)), RAT(yf, VAT2(iz, 9,lev-1)), RAT(zf, VAT2(iz,
00141 10,lev-1)));
00142
00143                 // Differential operator this level with standard disc.
00144                 if (*mgcoar == 0) {
00145
00146                     // Some i/o
00147                     if (*iinfo > 0)
00148                         VMESAGE3("Stand: (%03d, %03d, %03d)", nxx, nyy, nzz);
00149
00150
00151                     Vbuildcopy0(&nxx, &nyy, &nzz,
00152                         &nxold, &nyold, &nzold,
00153                         RAT(xf, VAT2(iz, 8,lev )), RAT(yf, VAT2(iz, 9,lev )), RAT(zf, VAT2(iz,
00154 10,lev )),
00155                         RAT(gxcf, VAT2(iz, 2,lev )), RAT(gycf, VAT2(iz, 3,lev )), RAT(gzcf, VAT2(iz,
00156 4,lev )),
00157                         RAT(alcf, VAT2(iz, 1,lev )), RAT(a2cf, VAT2(iz, 1,lev )), RAT(a3cf, VAT2(iz,
00158 1,lev )),
00159                         RAT(ccf, VAT2(iz, 1,lev )), RAT(fcf, VAT2(iz, 1,lev )), RAT(tcf, VAT2(iz,
00160 1,lev )),
00161                         RAT(xf, VAT2(iz, 8,lev-1)), RAT(yf, VAT2(iz, 9,lev-1)), RAT(zf, VAT2(iz,
00162 10,lev-1)),
00163                         RAT(gxcf, VAT2(iz, 2,lev-1)), RAT(gycf, VAT2(iz, 3,lev-1)), RAT(gzcf, VAT2(iz,
00164 4,lev-1)),
00165                         RAT(alcf, VAT2(iz, 1,lev-1)), RAT(a2cf, VAT2(iz, 1,lev-1)), RAT(a3cf, VAT2(iz,
00166 1,lev-1)),
00167                         RAT(ccf, VAT2(iz, 1,lev-1)), RAT(fcf, VAT2(iz, 1,lev-1)), RAT(tcf, VAT2(iz,
00168 1,lev-1)));
00169
00170                     VbuildA(&nxx, &nyy, &nzz,
00171                         ipkey, mgdisc, &numdia,
00172                         RAT(ipc, VAT2(iz, 5,lev)), RAT(rpc, VAT2(iz, 6,lev)),
00173                         RAT(ac, VAT2(iz, 7,lev)), RAT(cc, VAT2(iz, 1,lev)), RAT(fc, VAT2(iz,
00174 1,lev)),
00175                         RAT(xf, VAT2(iz, 8,lev)), RAT(yf, VAT2(iz, 9,lev)), RAT(zf, VAT2(iz,
00176 10,lev)),
00177                         RAT(gxcf, VAT2(iz, 2,lev)), RAT(gycf, VAT2(iz, 3,lev)), RAT(gzcf, VAT2(iz,
00178 4,lev)),
00179                         RAT(alcf, VAT2(iz, 1,lev)), RAT(a2cf, VAT2(iz, 1,lev)), RAT(a3cf, VAT2(iz,
00180 1,lev)),
00181                         RAT(ccf, VAT2(iz, 1,lev)), RAT(fcf, VAT2(iz, 1,lev)));
00182
00183                 }
00184
00185                 // Differential operator this level with harmonic disc.
00186                 else if (*mgcoar == 1) {
00187
00188                     // Some i/o
00189                     if (*iinfo > 0)
00190                         VMESAGE3("Harm0: (%03d, %03d, %03d)", nxx, nyy, nzz);
00191
00192                     Vbuildharm0(&nxx, &nyy, &nzz, &nxold, &nyold, &nzold,
00193                         RAT(xf, VAT2(iz, 8, lev )), RAT(yf, VAT2(iz, 9, lev )), RAT(zf,
00194 VAT2(iz, 10, lev )),
00195                         RAT(gxcf, VAT2(iz, 2, lev )), RAT(gycf, VAT2(iz, 3, lev )), RAT(gzcf,
00196 VAT2(iz, 4, lev )),
00197                         RAT(alcf, VAT2(iz, 1, lev )), RAT(a2cf, VAT2(iz, 1, lev )), RAT(a3cf,
00198 VAT2(iz, 1, lev )),
00199                         RAT(ccf, VAT2(iz, 1, lev )), RAT(fcf, VAT2(iz, 1, lev )), RAT(tcf,

```

```

    VAT2(iz, 1, lev )),
00184          RAT(xf, VAT2(iz, 8, lev-1)),  RAT(yf, VAT2(iz, 9, lev-1)),  RAT(zf,
    VAT2(iz, 10, lev-1)),
00185          RAT(gxcf, VAT2(iz, 2, lev-1)), RAT(gycf, VAT2(iz, 3, lev-1)), RAT(gzcf,
    VAT2(iz, 4, lev-1)),
00186          RAT(alcf, VAT2(iz, 1, lev-1)), RAT(a2cf, VAT2(iz, 1, lev-1)), RAT(a3cf,
    VAT2(iz, 1, lev-1)),
00187          RAT(ccf, VAT2(iz, 1, lev-1)),  RAT(fcf, VAT2(iz, 1, lev-1)),  RAT(tcf,
    VAT2(iz, 1, lev-1));
00188
00189      VbuildA(&nxx, &nyy, &nzz,
00190          ipkey, mgdisc, &numdia,
00191          RAT(ipc, VAT2(iz, 5,lev)),  RAT(rpc, VAT2(iz, 6,lev)),
00192          RAT(ac, VAT2(iz, 7,lev)),  RAT(cc, VAT2(iz, 1,lev)),  RAT(fc, VAT2(iz,
    1,lev)),
00193          RAT(xf, VAT2(iz, 8,lev)),  RAT(yf, VAT2(iz, 9,lev)),  RAT(zf, VAT2(iz,
    10,lev)),
00194          RAT(gxcf, VAT2(iz, 2,lev)), RAT(gycf, VAT2(iz, 3,lev)), RAT(gzcf, VAT2(iz,
    4,lev)),
00195          RAT(alcf, VAT2(iz, 1,lev)), RAT(a2cf, VAT2(iz, 1,lev)), RAT(a3cf, VAT2(iz,
    1,lev)),
00196          RAT(ccf, VAT2(iz, 1,lev)),  RAT(fcf, VAT2(iz, 1,lev)));
00197      }
00198
00199      // Differential operator with galerkin formulation ***
00200      else if (*mgcoar == 2) {
00201
00202          // Some i/o
00203          if (*iinfo > 0)
00204              VMESSAGE3("Galer: (%03d, %03d, %03d)", nxx, nyy, nzz);
00205
00206          Vbuildgaler0(&nxold, &nyold, &nzold,
00207              &nxx, &nyy, &nzz,
00208              ipkey, &numdia,
00209              RAT(pc, VAT2(iz, 11,lev-1)),
00210              RAT(ipc, VAT2(iz, 5,lev-1)), RAT(rpc, VAT2(iz, 6,lev-1)),
00211              RAT(ac, VAT2(iz, 7,lev-1)),  RAT(cc, VAT2(iz, 1,lev-1)), RAT(fc, VAT2(iz,
    1,lev-1)),
00212              RAT(ipc, VAT2(iz, 5,lev )), RAT(rpc, VAT2(iz, 6,lev )),
00213              RAT(ac, VAT2(iz, 7,lev )),  RAT(cc, VAT2(iz, 1,lev )), RAT(fc, VAT2(iz,
    1,lev  )));
00214
00215
00216
00217          Vextrac(&nxold, &nyold, &nzold,
00218              &nxx, &nyy, &nzz,
00219              RAT(tcf, VAT2(iz, 1,lev-1)), RAT(tcf, VAT2(iz, 1,lev)));
00220      }
00221      else {
00222          VABORT_MSG1("Bad mgcoar value given: %d", *mgcoar);
00223      }
00224
00225      // Now initialize the differential operator offset
00226      // Vnm_print(0, "BUILDOPS: operator stencil (lev,numdia) = (%d, %d)\n",
00227      // lev,numdia);
00228      VAT2(iz, 7, lev+1) = VAT2(iz, 7,lev) + numdia * nxx * nyy * nzz;
00229
00230      // Debug
00231      if (*iinfo > 8) {
00232
00233          Vprtmatd(&nxx, &nyy, &nzz,
00234              RAT(ipc, VAT2(iz, 5,lev)), RAT(rpc, VAT2(iz, 6,lev)), RAT(ac, VAT2(iz,
    7,lev)));
00235      }
00236      }
00237      }
00238
00239      // Build a sparse format coarse grid operator
00240      if (*mgsolv == 1) {
00241          lev = *nlev;
00242
00243          Vbuildband(&key, &nxx, &nyy, &nzz,
00244              RAT(ipc, VAT2(iz, 5,lev )), RAT(rpc, VAT2(iz, 6,lev )), RAT(ac, VAT2(iz, 7,lev )),
00245              RAT(ipc, VAT2(iz, 5,lev+1)), RAT(rpc, VAT2(iz, 6,lev+1)), RAT(ac, VAT2(iz, 7,lev+1)));
00246
00247          if (key == 1) {
00248              VERMSG0("Changing your mgsolv to iterative");
00249              *mgsolv = 0;
00250          }
00251      }
00252      }

```



```

00253 }
00254
00255
00256
00257 VPUBLIC void Vbuildstr(int *nx, int *ny, int *nz, int *nlev, int *iz) {
00258
00259     int nxold, nyold, nzold;
00260     int nxnew, nynew, nznew;
00261     int n, lev;
00262
00263     // Utility variable
00264     int numlev;
00265
00266     MAT2(iz, 50, *nlev);
00267
00268     // Setup
00269     nxnew = *nx;
00270     nynew = *ny;
00271     nznew = *nz;
00272     n      = nxnew * nynew * nznew;
00273
00274     // Start with level 1
00275     lev = 1;
00276
00277     // Mark beginning of everything at level 1 ***
00278     VAT2(iz, 1, lev) = 1;
00279     VAT2(iz, 2, lev) = 1;
00280     VAT2(iz, 3, lev) = 1;
00281     VAT2(iz, 4, lev) = 1;
00282     VAT2(iz, 5, lev) = 1;
00283     VAT2(iz, 6, lev) = 1;
00284     VAT2(iz, 7, lev) = 1;
00285     VAT2(iz, 8, lev) = 1;
00286     VAT2(iz, 9, lev) = 1;
00287     VAT2(iz, 10, lev) = 1;
00288     VAT2(iz, 11, lev) = 1;
00289
00290     // Mark beginning of everything at level 2
00291     VAT2(iz, 1, lev + 1) = VAT2(iz, 1, lev) + n;
00292     VAT2(iz, 2, lev + 1) = VAT2(iz, 2, lev) + 4 * nynew * nznew;
00293     VAT2(iz, 3, lev + 1) = VAT2(iz, 3, lev) + 4 * nxnew * nznew;
00294     VAT2(iz, 4, lev + 1) = VAT2(iz, 4, lev) + 4 * nxnew * nynew;
00295     VAT2(iz, 5, lev + 1) = VAT2(iz, 5, lev) + 100;
00296     VAT2(iz, 6, lev + 1) = VAT2(iz, 6, lev) + 100;
00297     VAT2(iz, 8, lev + 1) = VAT2(iz, 8, lev) + nxnew;
00298     VAT2(iz, 9, lev + 1) = VAT2(iz, 9, lev) + nynew;
00299     VAT2(iz, 10, lev + 1) = VAT2(iz, 10, lev) + nznew;
00300
00301     /* *****
00302     * ***NOTE: we mark operator offsets as we build the operators ***
00303     * ***VAT2(iz, 7,lev+1) = VAT2(iz, 7, lev) + 4*n ***
00304     * *****
00305     * ***NOTE: we mark prolongation operator offsets lagging a level ***
00306     * ***VAT2(iz, 11, lev) = VAT2(iz, 11,lev-1) + 27*nsmall ***
00307     * *****/
00308
00309     // Mark the beginning of everything at (nlev-1) more
00310     for (lev=2; lev<=*nlev; lev++) {
00311         nxold = nxnew;
00312         nyold = nynew;
00313         nzold = nznew;
00314         numlev = 1;
00315         Vmkcors(&numlev, &nxold, &nyold, &nzold, &nxnew, &nynew, &nznew);
00316         n = nxnew * nynew * nznew;
00317
00318         // Mark the beginning of everything at level (lev+1)
00319         VAT2(iz, 1, lev + 1) = VAT2(iz, 1, lev) + n;
00320         VAT2(iz, 2, lev + 1) = VAT2(iz, 2, lev) + 4 * nynew * nznew;
00321         VAT2(iz, 3, lev + 1) = VAT2(iz, 3, lev) + 4 * nxnew * nznew;
00322         VAT2(iz, 4, lev + 1) = VAT2(iz, 4, lev) + 4 * nxnew * nynew;
00323         VAT2(iz, 5, lev + 1) = VAT2(iz, 5, lev) + 100;
00324         VAT2(iz, 6, lev + 1) = VAT2(iz, 6, lev) + 100;
00325         VAT2(iz, 7, lev + 1) = VAT2(iz, 7, lev) + 4 * n;
00326         VAT2(iz, 8, lev + 1) = VAT2(iz, 8, lev) + nxnew;
00327         VAT2(iz, 9, lev + 1) = VAT2(iz, 9, lev) + nynew;
00328         VAT2(iz, 10, lev + 1) = VAT2(iz, 10, lev) + nznew;
00329
00330         // Mark prolongation operator storage for previous level
00331         VAT2(iz, 11, lev) = VAT2(iz, 11, lev - 1) + 27 * n;
00332
00333         /* *****

```

```

00334      * *** NOTE: we mark operator offsets as we build the operators ***
00335      * ***      VAT2(iz, 7, lev + 1) = VAT2(iz, 7, lev) + 4 * n ***
00336      * *****/
00337    }
00338  }
00339
00340
00341  VPUBLIC void Vbuildgaler0(int *nxf, int *nyf, int *nzf,
00342      int *nxc, int *nyc, int *nzc,
00343      int *ipkey, int *numdia,
00344      double *pcFF, int *ipcFF, double *rpcFF,
00345      double *acFF, double *ccFF, double *fcFF,
00346      int *ipc, double *rpc,
00347      double *ac, double *cc, double *fc) {
00348
00349      int numdia_loc;
00350
00351      // Call the algebraic galerkin routine
00352      numdia_loc = VAT(ipcFF, 11);
00353      VbuildG(nxf, nyf, nzf,
00354          nxc, nyc, nzc,
00355          &numdia_loc,
00356          pcFF, acFF, ac);
00357
00358      // Note how many nonzeros in this new discretization stencil
00359      VAT(ipc, 11) = 27;
00360      *numdia = 14;
00361
00362      // Save the problem key with this new operator
00363      VAT(ipc, 10) = *ipkey;
00364
00365      // Restrict the helmholtz term and source function
00366      Vrestrc(nxf, nyf, nzf,
00367          nxc, nyc, nzc,
00368          ccFF, cc, pcFF);
00369
00370      Vrestrc(nxf, nyf, nzf,
00371          nxc, nyc, nzc,
00372          fcFF, fc, pcFF);
00373  }
00374
00375
00376
00377  VPUBLIC void Vmkcors(int *numlev,
00378      int *nxold, int *nyold, int *nzold,
00379      int *nxnew, int *nynew, int *nznew) {
00380      int ntmp, nytmp, nztmp; // Temporary variables to hold current x,y,z values
00381      int i;                // Index used in for loops
00382
00383      // Determine the coarser grid
00384      *nxnew = *nxold;
00385      *nynew = *nyold;
00386      *nznew = *nzold;
00387
00388      for (i=1; i<=*numlev; i++) {
00389          ntmp = *nxnew;
00390          nytmp = *nynew;
00391          nztmp = *nznew;
00392          Vcorsr(&ntmp, nxnew);
00393          Vcorsr(&nytmp, nynew);
00394          Vcorsr(&nztmp, nznew);
00395      }
00396  }
00397
00398
00399
00400  VPUBLIC void Vcorsr(int *nold, int *nnew) {
00401
00402      // Find the coarser grid size ***
00403      *nnew = (*nold - 1) / 2 + 1;
00404
00405      // Check a few things
00406      if ((*nnew - 1) * 2 != *nold - 1) {
00407          Vnm_print(2, "Vcorsr: WARNING! The grid dimensions are not\n");
00408          Vnm_print(2, "Vcorsr: consistent with nlev! Your\n");
00409          Vnm_print(2, "Vcorsr: calculation will only work if you\n");
00410          Vnm_print(2, "Vcorsr: are performing a mg-dummy run.\n");
00411      }
00412      if (*nnew < 1) {
00413          Vnm_print(2, "Vcorsr: ERROR! The grid dimensions are not\n");
00414          Vnm_print(2, "Vcorsr: consistent with nlev!\n");
00415      }

```

```

00416         Vnm_print(2, "Vcorsr:  Grid coarsened below zero.\n");
00417     }
00418 }
00419
00420
00421
00422 VPUBLIC void Vmkfine(int *numlev,
00423     int *nxold, int *nyold, int *nzold,
00424     int *nxnew, int *nynew, int *nznew) {
00425
00426     int nxtmp, nytmp, nztmp, i;
00427
00428     // Determine the finer grid
00429     *nxnew = *nxold;
00430     *nynew = *nyold;
00431     *nznew = *nzold;
00432
00433     for (i=1; i<=*numlev; i++) {
00434
00435         nxtmp = *nxnew;
00436         nytmp = *nynew;
00437         nztmp = *nznew;
00438
00439         Vfiner(&nxtmp, nxnew);
00440         Vfiner(&nytmp, nynew);
00441         Vfiner(&nztmp, nznew);
00442     }
00443
00444 }
00445
00446
00447
00448 VPUBLIC void Vfiner(int *nold, int *nnew) {
00449     // Find the coarser grid size ***
00450     *nnew = (*nold - 1) * 2 + 1;
00451 }
00452
00453
00454
00455 VPUBLIC int Vivariv(int *nu, int *level) {
00456
00457     int ivariv;
00458
00459     // Variable V-cycle
00460     // ivariv = *nu * VPOW(2, level - 1);
00461
00462     // Standard V-cycle
00463     ivariv = *nu;
00464
00465     return ivariv;
00466 }
00467
00468
00469
00470
00471 VPUBLIC int Vmaxlev(int n1, int n2, int n3) {
00472
00473     int n1c;
00474     int n2c;
00475     int n3c;
00476     int lev;
00477     int iden;
00478     int idone;
00479
00480     // Fine the common level
00481     idone = 0;
00482     lev = 0;
00483     do {
00484         lev += 1;
00485         iden = (int)VPOW(2, lev - 1);
00486         n1c = (n1 - 1) / iden + 1;
00487         n2c = (n2 - 1) / iden + 1;
00488         n3c = (n3 - 1) / iden + 1;
00489         if ((n1c - 1) * iden != (n1 - 1)) || (n1c <= 2) )
00490             idone = 1;
00491         if ((n2c - 1) * iden != (n2 - 1)) || (n2c <= 2) )
00492             idone = 1;
00493         if ((n3c - 1) * iden != (n3 - 1)) || (n3c <= 2) )
00494             idone = 1;
00495     } while (idone != 1);
00496
00497

```

```

00498     return lev - 1;
00499 }
00500
00501
00502
00503 VPUBLIC void Vprtstp(int iok, int iters,
00504     double rsnrm, double rsden, double orsnrm) {
00505
00506     double relres = 0.0;
00507     double contrac = 0.0;
00508
00509     // Initializing timer
00510     if (iters == -99) {
00511         // Vnm_tstart(40, "MG iteration");
00512         cputme = 0.0;
00513         return;
00514     }
00515
00516     // Setup for the iteration
00517     else if (iters == -1) {
00518         Vnm_tstop(40, "MG iteration");
00519         return;
00520     }
00521
00522     // During the iteration
00523     else {
00524
00525         // Stop the timer
00526         // Vnm_tstop(40, "MG iteration");
00527
00528         // Relative residual
00529         if (rsden == 0.0) {
00530             relres = 1.0e6;
00531             VERRMSG0("Vprtstp: avoided division by zero\n");
00532         } else {
00533             relres = rsnrm / rsden;
00534         }
00535
00536         // Contraction number
00537         if (orsnrm == 0.0) {
00538             contrac = 1.0e6;
00539             VERRMSG0("avoided division by zero\n");
00540         } else {
00541             contrac = rsnrm / orsnrm;
00542         }
00543
00544         // The i/o
00545         if (iok == 1 || iok == 2) {
00546             VMESAGE1("iteration = %d", iters);
00547             VMESAGE1("relative residual = %e", relres);
00548             VMESAGE1("contraction number = %e", contrac);
00549         }
00550     }
00551 }
00552
00553
00554
00555 VPUBLIC void Vpackmg(int *iparm, double *rparm, size_t *nrwk, int *niwk,
00556     int *nx, int *ny, int *nz, int *nlev, int *nul, int *nu2, int *mgkey,
00557     int *itmax, int *istop, int *ipcon, int *nonlin, int *mgsmoo, int *mgprol,
00558     int *mgcoar, int *mgsolv, int *mgdisc, int *iinfo, double *errtol,
00559     int *ipkey, double *omegal, double *omegan, int *irite, int *iperf) {
00560
00561
00562
00563     // Encode iparm parameters ***
00564     VAT(iparm, 1) = *nrwk;
00565     VAT(iparm, 2) = *niwk;
00566     VAT(iparm, 3) = *nx;
00567     VAT(iparm, 4) = *ny;
00568     VAT(iparm, 5) = *nz;
00569     VAT(iparm, 6) = *nlev;
00570     VAT(iparm, 7) = *nul;
00571     VAT(iparm, 8) = *nu2;
00572     VAT(iparm, 9) = *mgkey;
00573     VAT(iparm, 10) = *itmax;
00574     VAT(iparm, 11) = *istop;
00575     VAT(iparm, 12) = *iinfo;
00576     VAT(iparm, 13) = *irite;
00577     VAT(iparm, 14) = *ipkey;
00578     VAT(iparm, 15) = *ipcon;
00579     VAT(iparm, 16) = *nonlin;

```

```

00580     VAT(iparm, 17) = *mgprol;
00581     VAT(iparm, 18) = *mgcoar;
00582     VAT(iparm, 19) = *mgdisc;
00583     VAT(iparm, 20) = *mgsmoo;
00584     VAT(iparm, 21) = *mgsolv;
00585     VAT(iparm, 22) = *iperf;
00586
00587     // Encode rparm parameters
00588     VAT(rparm, 1) = *errtol;
00589     VAT(rparm, 9) = *omegal;
00590     VAT(rparm, 10) = *omegan;
00591 }
00592
00593
00594
00595 VEXTERNC void Vbuildcopy0(int *nx, int *ny, int *nz,
00596     int *nxf, int *nyf, int *nzf,
00597     double *xc, double *yc, double *zc,
00598     double *gxc, double *gyc, double *gzc,
00599     double *alc, double *a2c, double *a3c,
00600     double *cc, double *fc, double *tc,
00601     double *xf, double *yf, double *zf,
00602     double *gxcf, double *gycf, double *gzcf,
00603     double *alcf, double *a2cf, double *a3cf,
00604     double *ccf, double *fcf, double *tcf) {
00605
00606
00607     int i, j, k;
00608     int ii, jj, kk;
00609     int iadd, jadd, kadd;
00610
00611     MAT3( gxc, *ny, *nz, 4);
00612     MAT3( gyc, *nx, *nz, 4);
00613     MAT3( gzc, *nx, *ny, 4);
00614     MAT3( alc, *nx, *ny, *nz);
00615     MAT3( a2c, *nx, *ny, *nz);
00616     MAT3( a3c, *nx, *ny, *nz);
00617     MAT3( cc, *nx, *ny, *nz);
00618     MAT3( fc, *nx, *ny, *nz);
00619     MAT3( tc, *nx, *ny, *nz);
00620     MAT3(gxcf, *nyf, *nzf, 4);
00621     MAT3(gycf, *nxf, *nzf, 4);
00622     MAT3(gzcf, *nxf, *nyf, 4);
00623     MAT3(alcf, *nxf, *nyf, *nzf);
00624     MAT3(a2cf, *nxf, *nyf, *nzf);
00625     MAT3(a3cf, *nxf, *nyf, *nzf);
00626     MAT3( tcf, *nxf, *nyf, *nzf);
00627     MAT3( ccf, *nxf, *nyf, *nzf);
00628     MAT3( fcf, *nxf, *nyf, *nzf);
00629
00630     WARN_UNTESTED;
00631
00632     // How far to step into the coefficient arrays
00633     iadd = (*nxf - 1) / (*nx - 1);
00634     jadd = (*nyf - 1) / (*ny - 1);
00635     kadd = (*nzf - 1) / (*nz - 1);
00636
00637     if (iadd != 2 || jadd != 2 || kadd != 2) {
00638         Vnm_print(2, "Vbuildcopy0: Problem with grid dimensions...\n");
00639     }
00640
00641     // Compute the coarse grid pde coefficients
00642     for (k=1; k<=*nz; k++) {
00643         kk = 2 * k - 1;
00644         VAT(zc, k) = VAT(zf, kk);
00645
00646         for (j=1; j<=*ny; j++) {
00647             jj = 2 * j - 1;
00648             VAT(yc, j) = VAT(yf, jj);
00649
00650             for (i=1; i<=*nx; i++){
00651                 ii = 2 * i - 1;
00652                 VAT(xc, i) = VAT(xf, ii);
00653
00654                 // True solution
00655                 VAT3( tc, i, j, k) = VAT3( tcf, ii, jj, kk);
00656
00657                 // Helmholtz coefficient
00658                 VAT3( cc, i, j, k) = VAT3( ccf, ii, jj, kk);
00659
00660                 // Source function

```

```

00661         VAT3( fc, i, j, k) = VAT3( fcf, ii, jj, kk);
00662
00663         // East/West neighbor
00664         VAT3(alc, i, j, k) = VAT3(alcf, ii, jj, kk);
00665
00666         // North/South neighbor
00667         VAT3(a2c, i, j, k) = VAT3(a2cf, ii, jj, kk);
00668
00669         // Up/Down neighbor
00670         VAT3(a3c, i, j, k) = VAT3(a3cf, ii, jj, kk);
00671     }
00672 }
00673 }
00674
00675 // The (i=1) and (i=nx) boundaries
00676 for (k=1; k<=*nz; k++) {
00677     kk = 2 * k - 1;
00678
00679     for (j=1; j<=*ny; j++) {
00680         jj = 2 * j - 1;
00681
00682         VAT3(gxc, j, k, 1) = VAT3(gxcf, jj, kk, 1);
00683         VAT3(gxc, j, k, 2) = VAT3(gxcf, jj, kk, 2);
00684         VAT3(gxc, j, k, 3) = VAT3(gxcf, jj, kk, 3);
00685         VAT3(gxc, j, k, 4) = VAT3(gxcf, jj, kk, 4);
00686     }
00687 }
00688
00689 // The (j=1) and (j=ny) boundaries
00690 for (k=1; k<=*nz; k++) {
00691     kk = 2 * k - 1;
00692
00693     for (i=1; i<=*nx; i++) {
00694         ii = 2 * i - 1;
00695
00696         VAT3(gyc, i, k, 1) = VAT3(gycf, ii, kk, 1);
00697         VAT3(gyc, i, k, 2) = VAT3(gycf, ii, kk, 2);
00698         VAT3(gyc, i, k, 3) = VAT3(gycf, ii, kk, 3);
00699         VAT3(gyc, i, k, 4) = VAT3(gycf, ii, kk, 4);
00700     }
00701 }
00702
00703 // The (k=1) and (k=nz) boundaries
00704 for (j=1; j<=*ny; j++) {
00705     jj = 2 * j - 1;
00706
00707     for (i=1; i<=*nx; i++) {
00708         ii = 2 * i - 1;
00709
00710         VAT3(gzc, i, j, 1) = VAT3(gzcf, ii, jj, 1);
00711         VAT3(gzc, i, j, 2) = VAT3(gzcf, ii, jj, 2);
00712         VAT3(gzc, i, j, 3) = VAT3(gzcf, ii, jj, 3);
00713         VAT3(gzc, i, j, 4) = VAT3(gzcf, ii, jj, 4);
00714     }
00715 }
00716 }
00717
00718 VPUBLIC void Vbuildharm0(int *nx, int *ny, int *nz,
00719     int *nxf, int *nyf, int *nzf,
00720     double *xc, double *yc, double *zc,
00721     double *gxc, double *gyc, double *gzc,
00722     double *alc, double *a2c, double *a3c,
00723     double *cc, double *fc, double *tc,
00724     double *xf, double *yf, double *zf,
00725     double *gxcf, double *gycf, double *gzcf,
00726     double *alcf, double *a2cf, double *a3cf,
00727     double *ccf, double *fcf, double *tcf) {
00728     #if 1
00729     Vnm_print(2, "WARNING:  FUNCTION IS NOT FULLY IMPLEMENTED YET!!!");
00730     #else
00731     int i, j, k;
00732     int ii, jj, kk;
00733     int iadd, jadd, kadd;
00734
00735     MAT3( gxc, *ny, *nz, 4);
00736     MAT3( gyc, *nx, *nz, 4);
00737     MAT3( gzc, *nx, *ny, 4);
00738
00739     MAT3( alc, *nx, *ny, *nz);
00740     MAT3( a2c, *nx, *ny, *nz);
00741     MAT3( a3c, *nx, *ny, *nz);

```

```

00742
00743     MAT3( cc, *nx, *ny, *nz);
00744     MAT3( fc, *nx, *ny, *nz);
00745     MAT3( tc, *nx, *ny, *nz);
00746
00747     MAT3(gxcf, *nyf, *nzf, 4);
00748     MAT3(gycf, *nxf, *nzf, 4);
00749     MAT3(gzcf, *nxf, *nyf, 4);
00750     MAT3(alcf, *nxf, *nyf, *nzf);
00751     MAT3(a2cf, *nxf, *nyf, *nzf);
00752     MAT3(a3cf, *nxf, *nyf, *nzf);
00753     MAT3( tcf, *nxf, *nyf, *nzf);
00754     MAT3( ccf, *nxf, *nyf, *nzf);
00755     MAT3( fcf, *nxf, *nyf, *nzf);
00756
00757     // Statement functions
00759     double a, b, c, d, e, f, g, h;
00760
00761     // How far to step into the coefficient arrays
00762     iadd = (*nxf - 1) / (*nx - 1);
00763     jadd = (*nyf - 1) / (*ny - 1);
00764     kadd = (*nzf - 1) / (*nz - 1);
00765     if (iadd != 2 || jadd != 2 || kadd != 2) {
00766         Vnm_print(2, "BUILDHARM0: problem with grid dimensions...\n");
00767     }
00768
00769     // Compute the coarse grid pde coefficients
00770     for (k=1; k<=*nz; k++) {
00771         kk = 2 * k - 1;
00772         VAT(zc, k) = VAT(zf, kk);
00773
00774         for (j=1; j<=*ny; j++) {
00775             jj = 2 * j - 1;
00776             VAT(yc, j) = VAT(yf, jj);
00777
00778             for (i=1; i<=*nx; i++) {
00779                 ii = 2 * i - 1;
00780                 VAT(xc, i) = VAT(xf, ii);
00781
00782                 // True solution
00783                 VAT3(tc, i, j, k) = VAT3(tcf, ii, jj, kk);
00784
00785                 // Helmholtz coefficient
00786                 VAT3(cc, i, j, k) = VAT3(ccf, ii, jj, kk);
00787
00788                 /* Commented out in original fortran code
00789                 cc(i,j,k) = (
00790                     +0.5e0 * ccf(ii,jj,kk)
00791                     +0.5e0 * ARITH6( ccf(max0(1,ii-1),jj,kk),
00792                         ccf(min0(nxf,ii+1),jj,kk),
00793                         ccf(ii,max0(1,jj-1),kk),
00794                         ccf(ii,min0(nyf,jj+1),kk),
00795                         ccf(ii,jj,max0(nzf,kk-1)),
00796                         ccf(ii,jj,min0(nzf,kk+1)) )
00797                     )
00798                 */
00799
00800                 // Source function
00801                 VAT3(fc, i, j, k) = VAT3(fcf, ii, jj, kk);
00802                 /*
00803                 fc(i,j,k) = (
00804                     +0.5e0 * fcf(ii,jj,kk)
00805                     +0.5e0 * ARITH6( fcf(max0(1,ii-1),jj,kk),
00806                         fcf(min0(nxf,ii+1),jj,kk),
00807                         fcf(ii,max0(1,jj-1),kk),
00808                         fcf(ii,min0(nyf,jj+1),kk),
00809                         fcf(ii,jj,max0(nzf,kk-1)),
00810                         fcf(ii,jj,min0(nzf,kk+1)) )
00811                     )
00812                 */
00813
00814                 // East/West neighbor
00815                 VAT3(alc, i, j, k) = (
00816                     +0.500 * HARMO2(VAT3(alcf, ii, jj, kk),
00817                         VAT3(alcf, VMIN2(*nxf, ii+1), jj, kk))
00818                     +0.125 * HARMO2(VAT3(alcf, ii, jj, VMAX2(1, kk-1)),
00819                         VAT3(alcf, VMIN2(*nxf, ii+1), jj, VMAX2(1, kk-1)))
00820                     +0.125 * HARMO2(VAT3(alcf, ii, jj, VMIN2(*nzf, kk+1)),
00821                         VAT3(alcf, VMIN2(*nxf, ii+1), jj, VMIN2(*nzf, kk+1)))
00822                     +0.125 * HARMO2(VAT3(alcf, ii, VMAX2(1, jj-1), kk),
00823                         VAT3(alcf, VMIN2(*nxf, ii+1), VMAX2(1, jj-1), kk))

```

```

00824         +0.125 * HARMO2(VAT3(a1cf, ii, VMIN2(*nyf, jj+1), kk),
00825                         VAT3(a1cf, VMIN2(*nxf, ii+1), VMIN2(*nyf, jj+1), kk))
00826     );
00827
00828     // North/South neighbor
00829     VAT3(a2c, i, j, k) = (
00830         +0.500 * HARMO2(VAT3(a2cf, ii, jj, kk),
00831                         VAT3(a2cf, ii, VMIN2(*nyf, jj+1), kk))
00832         +0.125 * HARMO2(VAT3(a2cf, ii, jj, VMAX2(1, kk-1)),
00833                         VAT3(a2cf, ii, VMIN2(*nyf, jj+1), VMAX2(1, kk-1)))
00834         +0.125 * HARMO2(VAT3(a2cf, ii, jj, VMIN2(*nzf, kk+1)),
00835                         VAT3(a2cf, ii, VMIN2(*nyf, jj+1), VMIN2(*nzf, kk+1)))
00836         +0.125 * HARMO2(VAT3(a2cf, VMAX2(1, ii-1), jj, kk),
00837                         VAT3(a2cf, VMAX2(1, ii-1), VMIN2(*nyf, jj+1), kk))
00838         +0.125 * HARMO2(VAT3(a2cf, VMIN2(*nxf, ii+1), jj, kk),
00839                         VAT3(a2cf, VMIN2(*nxf, ii+1), VMIN2(*nyf, jj+1), kk))
00840     );
00841
00842     // Up/Down neighbor
00843     VAT3(a3c, i, j, k) = (
00844         +0.500 * HARMO2(VAT3(a3cf, ii, jj, kk),
00845                         VAT3(a3cf, ii, jj, VMIN2(*nzf, kk+1)))
00846         +0.125 * HARMO2(VAT3(a3cf, ii, VMAX2(1, jj-1), kk),
00847                         VAT3(a3cf, ii, VMAX2(1, jj-1), VMIN2(*nzf, kk+1)))
00848         +0.125 * HARMO2(VAT3(a3cf, ii, VMIN2(*nyf, jj+1), kk),
00849                         VAT3(a3cf, ii, VMIN2(*nyf, jj+1), VMIN2(*nzf, kk+1)))
00850         +0.125 * HARMO2(VAT3(a3cf, VMAX2(1, ii-1), jj, kk),
00851                         VAT3(a3cf, VMAX2(1, ii-1), jj, VMIN2(*nzf, kk+1)))
00852         +0.125 * HARMO2(VAT3(a3cf, VMIN2(*nxf, ii+1), jj, kk),
00853                         VAT3(a3cf, VMIN2(*nxf, ii+1), jj, VMIN2(*nzf, kk+1)))
00854     );
00855     }
00856 }
00857 }
00858
00859 // The (i=1) and (i=nx) boundaries ***
00860 for (k=1; k<=*nz; k++) {
00861     kk = 2 * k - 1;
00862
00863     for (j=1; j<=*ny; j++) {
00864         jj = 2 * j - 1;
00865
00866         VAT3(gxc, j, k, 1) = VAT3(gxcf, jj, kk, 1);
00867         VAT3(gxc, j, k, 2) = VAT3(gxcf, jj, kk, 2);
00868         VAT3(gxc, j, k, 3) = VAT3(gxcf, jj, kk, 3);
00869         VAT3(gxc, j, k, 4) = VAT3(gxcf, jj, kk, 4);
00870     }
00871 }
00872
00873 // The (j=1) and (j=ny) boundaries
00874 for (k=1; k<=*nz; k++) {
00875     kk = 2 * k - 1;
00876
00877     for (i=1; i<=*nx; i++) {
00878         ii = 2 * i - 1;
00879         VAT3(gyc, i, k, 1) = VAT3(gycf, ii, kk, 1);
00880         VAT3(gyc, i, k, 2) = VAT3(gycf, ii, kk, 2);
00881         VAT3(gyc, i, k, 3) = VAT3(gycf, ii, kk, 3);
00882         VAT3(gyc, i, k, 4) = VAT3(gycf, ii, kk, 4);
00883     }
00884 }
00885
00886 // The (k=1) and (k=nz) boundaries
00887 for (j=1; j<=*ny; j++) {
00888     jj = 2 * j - 1;
00889
00890     for (i=1; i<=*nx; i++) {
00891         ii = 2 * i - 1;
00892
00893         VAT3(gzc, i, j, 1) = VAT3(gzcf, ii, jj, 1);
00894         VAT3(gzc, i, j, 2) = VAT3(gzcf, ii, jj, 2);
00895         VAT3(gzc, i, j, 3) = VAT3(gzcf, ii, jj, 3);
00896         VAT3(gzc, i, j, 4) = VAT3(gzcf, ii, jj, 4);
00897     }
00898 }
00899 #endif
00900 }
00901
00902
00903
00904 VPUBLIC void Vbuildalg(int *nx, int *ny, int *nz,

```



```

00905     int *mode, int *nlev, int *iz,
00906     int *ipc, double *rpc,
00907     double *ac, double *cc, double *fc,
00908     double *x, double *y, double *tmp) {
00909
00910     int   nxx,   nyy,   nzz;
00911     int nxold, nyold, nzold;
00912     int lev, numlev;
00913
00914     MAT2(iz, 50, *nlev);
00915
00916     // Setup
00917     nxx = *nx;
00918     nyy = *ny;
00919     nzz = *nz;
00920
00921     // Build the rhs the finest level
00922     lev = 1;
00923     if ((*mode == 1) || (*mode == 2)) {
00924         Vnmatvec(&nxx, &nyy, &nzz,
00925                 RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00926                 RAT(ac, VAT2(iz, 7, lev)), RAT(cc, VAT2(iz, 1, lev)),
00927                 RAT(x, VAT2(iz, 1, lev)), RAT(y, VAT2(iz, 1, lev)),
00928                 tmp);
00929     } else {
00930         Vmatvec(&nxx, &nyy, &nzz,
00931                RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00932                RAT(ac, VAT2(iz, 7, lev)), RAT(cc, VAT2(iz, 1, lev)),
00933                RAT(x, VAT2(iz, 1, lev)), RAT(y, VAT2(iz, 1, lev)));
00934     }
00935
00936     // Build the (nlev-1) level rhs function
00937     for (lev=2; lev <= *nlev; lev++) {
00938         nxold = nxx;
00939         nyold = nyy;
00940         nzold = nzz;
00941
00942         numlev = 1;
00943         Vmkcors(&numlev, &nxold, &nyold, &nzold, &nxx, &nyy, &nzz);
00944
00945         // Build the rhs on this level
00946         if ((*mode == 1) || (*mode == 2)) {
00947             Vnmatvec(&nxx, &nyy, &nzz,
00948                     RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00949                     RAT(ac, VAT2(iz, 7, lev)), RAT(cc, VAT2(iz, 1, lev)),
00950                     RAT(x, VAT2(iz, 1, lev)), RAT(y, VAT2(iz, 1, lev)),
00951                     tmp);
00952         } else {
00953             Vmatvec(&nxx, &nyy, &nzz,
00954                    RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00955                    RAT(ac, VAT2(iz, 7, lev)), RAT(cc, VAT2(iz, 1, lev)),
00956                    RAT(x, VAT2(iz, 1, lev)), RAT(y, VAT2(iz, 1, lev)));
00957         }
00958     }
00959 }

```

9.135 mgsubd.h

```

00001
00050 #ifndef _MGSUBD_H_
00051 #define _MGSUBD_H_
00052
00053 #include "apbscfg.h"
00054
00055 #include "malloc/malloc.h"
00056
00057 #include "generic/vhal.h"
00058 #include "generic/vmatrix.h"
00059 #include "pmgc/matvecd.h"
00060 #include "pmgc/buildAd.h"
00061 #include "pmgc/buildPd.h"
00062 #include "pmgc/buildBd.h"
00063 #include "pmgc/buildGd.h"
00064
00065 #define HARMO2(a, b) ((2.0 * (a) * (b)) / ((a) + (b)))
00066 #define HARMO4(a, b, c, d) ((1.0 / (0.25 * (1.0/(a) + 1.0/(b) + 1.0/(c) + 1.0/(d))))
00067 #define ARITH2(a, b) ((a) + (b)) / 2.0
00068 #define ARITH4(a, b, c, d) ((a) + (b) + (c) + (d)) / 4.0

```

```

00069 #define ARITH6(a, b, c, d, e, f)      (((a) + (b) + (c) + (d) + (e) + (f)) / 6.0)
00070 #define ARITH8(a, b, c, d, e, f, g, h)  (((a) + (b) + (c) + (d) + (e) + (f) + (g) + (h)) / 8.0)
00071
00084 VEXTERNC void Vbuildops(
00085     int    *nx,
00086     int    *ny,
00087     int    *nz,
00088     int    *nlev,
00089     int    *ipkey,
00090     int    *iinfo,
00091     int    *ido,
00092     int    *iz,
00093     int    *mgprol,
00094     int    *mgcoar,
00095     int    *mgsolv,
00096     int    *mgdisc,
00097     int    *ipc,
00098     double *rpc,
00099     double *pc,
00100     double *ac,
00101     double *cc,
00102     double *fc,
00103     double *xf,
00104     double *yf,
00105     double *zf,
00106     double *gxcf,
00107     double *gycf,
00108     double *gzcf,
00109     double *alcf,
00110     double *a2cf,
00111     double *a3cf,
00112     double *ccf,
00113     double *fcf,
00114     double *tcf
00115 );
00116
00136 VEXTERNC void Vbuildstr(
00137     int    *nx,
00138     int    *ny,
00139     int    *nz,
00140     int    *nlev,
00141     int    *iz
00142 );
00143
00152 VEXTERNC void Vbuildgaler0(
00153     int    *nxf,
00154     int    *nyf,
00155     int    *nzf,
00156     int    *nxc,
00157     int    *nyc,
00158     int    *nzc,
00159     int    *ipkey,
00160     int    *numdia,
00161     double *pcFF,
00162     int    *ipcFF,
00163     double *rpcFF,
00164     double *acFF,
00165     double *ccFF,
00166     double *fcFF,
00167     int    *ipc,
00168     double *rpc,
00169     double *ac,
00170     double *cc,
00171     double *fc
00172 );
00173
00174
00175
00182 VEXTERNC void Vmkcors(
00183     int    *numlev,
00184     int    *nxold,
00185     int    *nyold,
00186     int    *nzold,
00187     int    *nxnew,
00188     int    *nynew,
00189     int    *nznew
00190 );
00191
00198 VEXTERNC void Vcorsr(
00199     int    *nold,
00200     int    *nnew

```

```
00201         );
00202
00203
00204
00211 VEXTERNC void Vmkfine(
00212     int *numlev,
00213     int *nxold,
00214     int *nyold,
00215     int *nzold,
00216     int *nxnew,
00217     int *nynew,
00218     int *nznew
00219 );
00220
00227 VEXTERNC void Vfiner(
00228     int *nold,
00229     int *nnew
00230 );
00231
00232
00233
00240 VEXTERNC int Vivariv(
00241     int *nu,
00242     int *level
00243 );
00244
00250 VEXTERNC int Vmaxlev(
00251     int n1,
00252     int n2,
00253     int n3
00254 );
00255
00256
00258 double bf, oh, cputme;
00259
00264 VEXTERNC void Vprtstp(
00265     int iok,
00266     int iters,
00267     double rsnm,
00268     double rsden,
00269     double orsnrm
00270 );
00271
00272
00273
00280 VEXTERNC void Vpackmg(
00281     int *iparm,
00282     double *rparm,
00283     size_t *nrwk,
00284     int *niwk,
00285     int *nx,
00286     int *ny,
00287     int *nz,
00288     int *nlev,
00289     int *nul,
00290     int *nu2,
00291     int *mgkey,
00292     int *itmax,
00293     int *istop,
00294     int *ipcon,
00295     int *nonlin,
00296     int *mgsmoo,
00297     int *mgprol,
00298     int *mgcoar,
00299     int *mgsolv,
00300     int *mgdisc,
00301     int *iinfo,
00302     double *errtol,
00303     int *ipkey,
00304     double *omegal,
00305     double *omegan,
00306     int *irite,
00307     int *iperf
00308 );
00309
00310
00311
00317 VEXTERNC void Vbuildharm0(
00318     int *nx,
00319     int *ny,
00320     int *nz,
```

```

00321         int *nxf,
00322         int *nyf,
00323         int *nzf,
00324         double *xc,
00325         double *yc,
00326         double *zc,
00327         double *gxc,
00328         double *gyc,
00329         double *gzc,
00330         double *alc,
00331         double *a2c,
00332         double *a3c,
00333         double *cc,
00334         double *fc,
00335         double *tc,
00336         double *xf,
00337         double *yf,
00338         double *zf,
00339         double *gxcf,
00340         double *gycf,
00341         double *gzcf,
00342         double *alcf,
00343         double *a2cf,
00344         double *a3cf,
00345         double *ccf,
00346         double *fcf,
00347         double *tcf
00348     );
00349
00350
00351
00357 VEXTERNC void Vbuildcopy0(
00358     int *nx,
00359     int *ny,
00360     int *nz,
00361     int *nxf,
00362     int *nyf,
00363     int *nzf,
00364     double *xc,
00365     double *yc,
00366     double *zc,
00367     double *gxc,
00368     double *gyc,
00369     double *gzc,
00370     double *alc,
00371     double *a2c,
00372     double *a3c,
00373     double *cc,
00374     double *fc,
00375     double *tc,
00376     double *xf,
00377     double *yf,
00378     double *zf,
00379     double *gxcf,
00380     double *gycf,
00381     double *gzcf,
00382     double *alcf,
00383     double *a2cf,
00384     double *a3cf,
00385     double *ccf,
00386     double *fcf,
00387     double *tcf
00388 );
00389
00390
00391
00397 VEXTERNC void Vbuildalg(
00398     int *nx,
00399     int *ny,
00400     int *nz,
00401     int *mode,
00402     int *nlev,
00403     int *iz,
00404     int *ipc,
00405     double *rpc,
00406     double *ac,
00407     double *cc,
00408     double *fc,
00409     double *x,
00410     double *y,
00411     double *tmp

```

```

00412 );
00413
00414
00415
00416 #endif // _MGSUBD_H_

```

9.136 mikpckd.c

```

00001
00055 #include "mikpckd.h"
00056
00057 VPUBLIC void Vxcopy(int *nx, int *ny, int *nz, double *x, double *y) {
00058
00059     MAT3(x, *nx, *ny, *nz);
00060     MAT3(y, *nx, *ny, *nz);
00061
00062     // The indices used to traverse the matrices
00063     int i, j, k;
00064
00066     #pragma omp parallel for private(i,j,k)
00067     for(k=2; k<=*nz-1; k++)
00068         for(j=2; j<=*ny-1; j++)
00069             for(i=2; i<=*nx-1; i++)
00070                 VAT3(y, i, j, k) = VAT3(x, i, j, k);
00071 }
00072
00073
00074
00075 VPUBLIC void Vxcopy_small(int *nx, int *ny, int *nz, double *x, double *y) {
00076
00077     MAT3(x, *nx, *ny, *nz);
00078     MAT3(y, *nx - 2, *ny - 2, *nz - 2);
00079
00080     // The indices used to traverse the matrices
00081     int i, j, k;
00082
00083     for(k=2; k<=*nz-1; k++)
00084         for(j=2; j<=*ny-1; j++)
00085             for(i=2; i<=*nx-1; i++)
00086                 VAT3(y, i - 1, j - 1, k - 1) = VAT3(x, i, j, k);
00087 }
00088
00089
00090
00091 VPUBLIC void Vxcopy_large(int *nx, int *ny, int *nz, double *x, double *y) {
00092
00093     MAT3(x, *nx - 2, *ny - 2, *nz - 2);
00094     MAT3(y, *nx, *ny, *nz);
00095
00096     // The indices used to traverse the matrices
00097     int i, j, k;
00098
00099     for(k=2; k<=*nz-1; k++)
00100         for(j=2; j<=*ny-1; j++)
00101             for(i=2; i<=*nx-1; i++)
00102                 VAT3(y, i, j, k) = VAT3(x, i - 1, j - 1, k - 1);
00103 }
00104
00105
00106
00107
00108
00109
00110
00111
00112 VPUBLIC void Vxaxpy(int *nx, int *ny, int *nz,
00113     double *alpha, double *x, double *y) {
00114
00115     // Create the wrappers
00116     MAT3(x, *nx, *ny, *nz);
00117     MAT3(y, *nx, *ny, *nz);
00118
00119     // The indices used to traverse the matrices
00120     int i, j, k;
00121
00122     for(k=2; k<=*nz-1; k++)
00123         for(j=2; j<=*ny-1; j++)
00124             for(i=2; i<=*nx-1; i++)
00125                 VAT3(y, i, j, k) += *alpha * VAT3(x, i, j, k);
00126 }
00127
00128
00129
00130

```

```

00131 VPUBLIC double Vxnrm1(int *nx, int *ny, int *nz,
00132     double *x) {
00133
00134     double xnrml = 0.0;
00135
00136     MAT3(x, *nx, *ny, *nz);
00137
00138     // The indices used to traverse the matrices
00139     int i, j, k;
00140
00142     for(k=2; k<=*nz-1; k++)
00143         for(j=2; j<=*ny-1; j++)
00144             for(i=2; i<=*nx-1; i++)
00145                 xnrml += VABS(VAT3(x, i, j, k));
00146
00147     return xnrml;
00148 }
00149
00150
00151
00152 VPUBLIC double Vxnrm2(int *nx, int *ny, int *nz,
00153     double *x) {
00154
00155     double xnrm2 = 0.0;
00156
00157     MAT3(x, *nx, *ny, *nz);
00158
00159     // The indices used to traverse the matrices
00160     int i, j, k;
00161
00163     for(k=2; k<=*nz-1; k++)
00164         for(j=2; j<=*ny-1; j++)
00165             for(i=2; i<=*nx-1; i++)
00166                 xnrm2 += VAT3(x, i, j, k) * VAT3(x, i, j, k);
00167
00168     return VSQRT(xnrm2);
00169 }
00170
00171
00172
00173 VPUBLIC double Vxdot(int *nx, int *ny, int *nz,
00174     double *x, double *y) {
00175
00176     int i, j, k;
00177
00178     // Initialize
00179     double xdot = 0.0;
00180
00181     MAT3(x, *nx, *ny, *nz);
00182     MAT3(y, *nx, *ny, *nz);
00183
00184     // Do it
00185     for(k=2; k<=*nz-1; k++)
00186         for(j=2; j<=*ny-1; j++)
00187             for(i=2; i<=*nx-1; i++)
00188                 xdot += VAT3(x, i, j, k) * VAT3(y, i, j, k);
00189
00190     return xdot;
00191 }
00192
00193
00194
00195 VPUBLIC void Vazeros(int *nx, int *ny, int *nz, double *x) {
00196
00197     int i, n;
00198     int nproc = 1;
00199
00200     n = *nx * *ny * *nz;
00201
00202     #pragma omp parallel for private(i)
00203     for (i=1; i<=n; i++)
00204         VAT(x, i) = 0.0;
00205 }
00206
00207
00208
00209 VPUBLIC void VfboundPMG(int *ibound, int *nx, int *ny, int *nz,
00210     double *x, double *gxc, double *gyc, double *gzc) {
00211
00212     int i, j, k;
00213

```

```

00214     // Create and bind the wrappers for the source data
00215     MAT3( x, *nx, *ny, *nz);
00216     MAT3(gxc, *ny, *nz, 2);
00217     MAT3(gyc, *nx, *nz, 2);
00218     MAT3(gzc, *nx, *ny, 2);
00219
00220     // Dirichlet test
00221     if (ibound == 0) {
00222
00223         // Dero dirichlet
00224         VfboundPMG00(nx, ny, nz, x);
00225
00226     } else {
00227
00228         // Nonzero dirichlet
00229
00230         // The (i=1) and (i=nx) boundaries
00231         for (k=1; k<=*nz; k++) {
00232             for (j=1; j<=*ny; j++) {
00233                 VAT3(x, 1, j, k) = VAT3(gxc, j, k, 1);
00234                 VAT3(x, *nx, j, k) = VAT3(gxc, j, k, 2);
00235             }
00236         }
00237
00238         // The (j=1) and (j=ny) boundaries
00239         for (k=1; k<=*nz; k++) {
00240             for (i=1; i<=*nx; i++) {
00241                 VAT3(x, i, 1, k) = VAT3(gyc, i, k, 1);
00242                 VAT3(x, i, *ny, k) = VAT3(gyc, i, k, 2);
00243             }
00244         }
00245
00246         // The (k=1) and (k=nz) boundaries
00247         for (j=1; j<=*ny; j++) {
00248             for (i=1; i<=*nx; i++) {
00249                 VAT3(x, i, j, 1) = VAT3(gzc, i, j, 1);
00250                 VAT3(x, i, j, *nz) = VAT3(gzc, i, j, 2);
00251             }
00252         }
00253     }
00254 }
00255
00256
00257
00258 VPUBLIC void VfboundPMG00(int *nx, int *ny, int *nz, double *x) {
00259
00260     int i, j, k;
00261
00262     MAT3( x, *nx, *ny, *nz);
00263
00264     // The (i=1) and (i=nx) boundaries
00265     for (k=1; k<=*nz; k++) {
00266         for (j=1; j<=*ny; j++) {
00267             VAT3(x, 1, j, k) = 0.0;
00268             VAT3(x, *nx, j, k) = 0.0;
00269         }
00270     }
00271
00272     // The (j=1) and (j=ny) boundaries
00273     for (k=1; k<=*nz; k++) {
00274         for(i=1; i<=*nx; i++) {
00275             VAT3(x, i, 1, k) = 0.0;
00276             VAT3(x, i, *ny, k) = 0.0;
00277         }
00278     }
00279
00280     // The (k=1) and (k=nz) boundaries
00281     for (j=1; j<=*ny; j++) {
00282         for (i=1; i<=*nx; i++) {
00283             VAT3(x, i, j, 1) = 0.0;
00284             VAT3(x, i, j, *nz) = 0.0;
00285         }
00286     }
00287 }
00288
00289
00290
00291 VPUBLIC void Vaxrand(int *nx, int *ny, int *nz, double *x) {
00292
00293     int n, i, ii, ipara, ivect, iflag;
00294     int nproc = 1;

```

```

00295     double xdum;
00296
00297     WARN_UNTESTED;
00298
00299     // Find parallel loops (ipara), remainder (ivect)
00300     n = *nx * *ny * *nz;
00301     ipara = n / nproc;
00302     ivect = n % nproc;
00303     iflag = 1;
00304     xdum = (double) (VRAND);
00305
00306     // Do parallel loops
00307     for (ii=1; ii<=nproc; ii++)
00308         for (i=1+(ipara*(ii-1)); i<=ipara*ii; i++)
00309             VAT(x, i) = (double) (VRAND);
00310
00311     // Do vector loops
00312     for (i=ipara*nproc+1; i<=n; i++)
00313         VAT(x, i) = (double) (VRAND);
00314 }
00315
00316
00317
00318 VPUBLIC void Vxscal(int *nx, int *ny, int *nz, double *fac, double *x) {
00319     int i, j, k;
00320
00321     MAT3(x, *nx, *ny, *nz);
00322
00323     for (k=2; k<=*nz-1; k++)
00324         for (j=2; j<=*ny-1; j++)
00325             for (i=2; i<=*nx-1; i++)
00326                 VAT3(x, i, j, k) *= *fac;
00327 }
00328
00329
00330
00331
00332 VPUBLIC void Vprtmtd(int *nx, int *ny, int *nz,
00333     int *ipc, double *rpc, double *ac) {
00334     int numdia;
00335
00336     MAT2(ac, *nx * *ny * *nz, 1);
00337
00338     WARN_UNTESTED;
00339
00340     // Do the printing
00341     numdia = VAT(ipc, 11);
00342     if (numdia == 7) {
00343         Vprtmtd7(nx, ny, nz,
00344             ipc, rpc,
00345             RAT2(ac, 1, 1), RAT2(ac, 1, 2), RAT2(ac, 1, 3), RAT2(ac, 1, 4));
00346     } else if (numdia == 27) {
00347         Vprtmtd27(nx, ny, nz,
00348             ipc, rpc,
00349             RAT2(ac, 1, 1), RAT2(ac, 1, 2), RAT2(ac, 1, 3), RAT2(ac, 1, 4),
00350             RAT2(ac, 1, 5), RAT2(ac, 1, 6),
00351             RAT2(ac, 1, 7), RAT2(ac, 1, 8), RAT2(ac, 1, 9), RAT2(ac, 1, 10),
00352             RAT2(ac, 1, 11), RAT2(ac, 1, 12), RAT2(ac, 1, 13), RAT2(ac, 1, 14));
00353     } else {
00354         Vnm_print(2, "Vprtmtd: invalid stencil type given: %d\n", numdia);
00355     }
00356 }
00357
00358
00359
00360
00361 VPUBLIC void Vprtmtd7(int *nx, int *ny, int *nz,
00362     int *ipc, double *rpc,
00363     double *oC, double *oE, double *oN, double *uC) {
00364     int n, i, j, k;
00365
00366     MAT3(oC, *nx, *ny, *nz);
00367     MAT3(oE, *nx, *ny, *nz);
00368     MAT3(oN, *nx, *ny, *nz);
00369     MAT3(uC, *nx, *ny, *nz);
00370
00371     WARN_UNTESTED;
00372
00373     // Recover matrix dimension
00374     n = (*nx - 2) * (*ny - 2) * (*nz - 2);

```



```

00376
00377     Vnm_print(2, "Vprtmatd7: Dimension of matrix = %d\n", n);
00378     Vnm_print(2, "Vprtmatd7: Begin diagonal matrix\n");
00379
00380     // Handle first block
00381     for (k=2; k<=*nz-1; k++)
00382         for (j=2; j<=*ny-1; j++)
00383             for (i=2; i<=*nx-1; i++)
00384                 Vnm_print(2, "Vprtmatd7: (%d,%d,%d) - oC=%g, oE=%g, oN=%g, uC=%g\n",
00385                     VAT3(oC,i,j,k), VAT3(oE,i,j,k), VAT3(oN,i,j,k), VAT3(uC,i,j,k));
00386
00387     // Finish up
00388     Vnm_print(2, "Vprtmatd7: End diagonal matrix\n");
00389 }
00390
00391
00392
00393 VEXTERNC void Vprtmatd27(int *nx, int *ny, int *nz,
00394     int *ipc, double *rpc,
00395     double *oC, double *oE, double *oN, double *uC,
00396     double *oNE, double *oNW,
00397     double *uE, double *uW, double *uN, double *uS,
00398     double *uNE, double *uNW, double *uSE, double *uSW) {
00399
00400     int n, i, j, k;
00401
00402     MAT3( oC, *nx, *ny, *nz);
00403     MAT3( oE, *nx, *ny, *nz);
00404     MAT3( oN, *nx, *ny, *nz);
00405     MAT3( uC, *nx, *ny, *nz);
00406     MAT3(oNE, *nx, *ny, *nz);
00407     MAT3(oNW, *nx, *ny, *nz);
00408     MAT3( uE, *nx, *ny, *nz);
00409     MAT3( uW, *nx, *ny, *nz);
00410     MAT3( uN, *nx, *ny, *nz);
00411     MAT3( uS, *nx, *ny, *nz);
00412     MAT3(uNE, *nx, *ny, *nz);
00413     MAT3(uNW, *nx, *ny, *nz);
00414     MAT3(uSE, *nx, *ny, *nz);
00415     MAT3(uSW, *nx, *ny, *nz);
00416
00417     WARN_UNTESTED;
00418
00419     // Recover matrix dimension
00420     n = (*nx - 2) * (*ny - 2) * (*nz - 2);
00421
00422     Vnm_print(2, "Vprtmatd27: Dimension of matrix = %d\n", n);
00423     Vnm_print(2, "Vprtmatd27: Begin diagonal matrix\n");
00424
00425     // Handle first block
00426     for (k=2; k<=*nz-1; k++)
00427         for (j=2; j<=*ny-1; j++)
00428             for (i=2; i<=*nx-1; i++)
00429                 Vnm_print(2, "Vprtmatd7: (%d,%d,%d) - oC = %g, oE = %g, "
00430                     "oNW = %g, oN = %g, oNE = %g, uSW = %g, uS = %g, "
00431                     "uSE = %g, uW = %g, uC = %g, uE = %g, uNW = %g, "
00432                     "uN = %g, uNE = %g\n",
00433                     VAT3( oC, i, j, k), VAT3( oE, i, j, k),
00434                     VAT3(oNW, i, j, k), VAT3( oN, i, j, k),
00435                     VAT3(oNE, i, j, k), VAT3(uSW, i, j, k),
00436                     VAT3( uS, i, j, k), VAT3(uSE, i, j, k),
00437                     VAT3( uW, i, j, k), VAT3( uC, i, j, k),
00438                     VAT3( uE, i, j, k), VAT3(uNW, i, j, k),
00439                     VAT3( uN, i, j, k), VAT3(uNE, i, j, k) );
00440
00441     // Finish up
00442     Vnm_print(2, "Vprtmatd27: End diagonal matrix\n");
00443 }
00444
00445 VPUBLIC void Vlinesearch(int *nx, int *ny, int *nz,
00446     double *alpha,
00447     int *ipc, double *rpc,
00448     double *ac, double *cc, double *fc,
00449     double *p, double *x, double *r,
00450     double *ap, double *zk, double *zkp1) {
00451     VABORT_MSG0("Not translated yet");
00452 }

```

9.137 mikpckd.h

```
00001
00050 #ifndef MIKPKKD_H_
00051 #define MIKPKKD_H_
00052
00053 #include "apbscfg.h"
00054
00055 #include "malloc/malloc.h"
00056
00057 #include "generic/vhal.h"
00058 #include "generic/vmatrix.h"
00059
00067 VEXTERNC void Vxcopy (
00068     int *nx,
00069     int *ny,
00070     int *nz,
00071     double *x,
00072     double *y
00073 );
00074
00075
00076
00084 VEXTERNC void Vxcopy_small (
00085     int *nx,
00086     int *ny,
00087     int *nz,
00088     double *x,
00089     double *y
00090 );
00091
00092
00093
00101 VEXTERNC void Vxcopy_large (
00102     int *nx,
00103     int *ny,
00104     int *nz,
00105     double *x,
00106     double *y
00107 );
00108
00109
00110
00117 VEXTERNC void Vxaxpy (
00118     int *nx,
00119     int *ny,
00120     int *nz,
00121     double *alpha,
00122     double *x,
00123     double *y
00124 );
00125
00132 VEXTERNC double Vxnrm1 (
00133     int *nx,
00134     int *ny,
00135     int *nz,
00136     double *x
00137 );
00138
00139
00140
00147 VEXTERNC double Vxnrm2 (
00148     int *nx,
00149     int *ny,
00150     int *nz,
00151     double *x
00152 );
00153
00160 VEXTERNC double Vxdot (
00161     int *nx,
00162     int *ny,
00163     int *nz,
00164     double *x,
00165     double *y
00166 );
00167
00174 VEXTERNC void Vazeros (
00175     int *nx,
00176     int *ny,
00177     int *nz,
```

```
00178         double *x
00179     );
00180
00187 VEXTERNC void VfboundPMG(
00188     int *ibound,
00189     int *nx,
00190     int *ny,
00191     int *nz,
00192     double *x,
00193     double *gxc,
00194     double *gyc,
00195     double *gzc
00196 );
00197
00204 VEXTERNC void VfboundPMG00(
00205     int *nx,
00206     int *ny,
00207     int *nz,
00208     double *x
00209 );
00210
00217 VEXTERNC void Vaxrand(
00218     int *nx,
00219     int *ny,
00220     int *nz,
00221     double *x
00222 );
00223
00230 VEXTERNC void Vxscal(
00231     int *nx,
00232     int *ny,
00233     int *nz,
00234     double *fac,
00235     double *x
00236 );
00237
00244 VEXTERNC void Vprtmatd(
00245     int *nx,
00246     int *ny,
00247     int *nz,
00248     int *ipc,
00249     double *rpc,
00250     double *ac
00251 );
00252
00253 VEXTERNC void Vprtmatd7(
00254     int *nx,
00255     int *ny,
00256     int *nz,
00257     int *ipc,
00258     double *rpc,
00259     double *oC,
00260     double *oE,
00261     double *oN,
00262     double *uC
00263 );
00264
00265 VEXTERNC void Vprtmatd27(
00266     int *nx,
00267     int *ny,
00268     int *nz,
00269     int *ipc,
00270     double *rpc,
00271     double *oC,
00272     double *oE,
00273     double *oN,
00274     double *uC,
00275     double *oNE,
00276     double *oNW,
00277     double *uE,
00278     double *uW,
00279     double *uN,
00280     double *uS,
00281     double *uNE,
00282     double *uNW,
00283     double *uSE,
00284     double *uSW
00285 );
00286
00287 VEXTERNC void Vlinesearch(
00288     int *nx,
```

```

00289         int      *ny,
00290         int      *nz,
00291         double   *alpha,
00292         int      *ipc,
00293         double   *rpc,
00294         double   *ac,
00295         double   *cc,
00296         double   *fc,
00297         double   *p,
00298         double   *x,
00299         double   *r,
00300         double   *ap,
00301         double   *zk,
00302         double   *zkip1
00303     );
00304
00305 #endif /* MIKPCCKD_H_ */

```

9.138 mlinpckd.c

```

00001
00055 #include "mlinpckd.h"
00056
00057 VPUBLIC void Vdpbs1(double *abd, int *lda, int *n, int *m, double *b) {
00058
00059     double t;
00060     int k, kb, la, lb, lm;
00061
00062     MAT2(abd, *lda, 1);
00063
00064     for (k=1; k<=*n; k++) {
00065         lm = VMIN2(k-1, *m);
00066         la = *m + 1 - lm;
00067         lb = k - lm;
00068         t = Vddot(lm, RAT2(abd, la, k), 1, RAT(b, lb), 1);
00069         VAT(b, k) = (VAT(b, k) - t) / VAT2(abd, *m+1, k);
00070     }
00071
00072     // Solve R*X = Y
00073     for (kb=1; kb<=*n; kb++) {
00074
00075         k = *n + 1 - kb;
00076         lm = VMIN2(k-1, *m);
00077         la = *m + 1 - lm;
00078         lb = k - lm;
00079         VAT(b, k) /= VAT2(abd, *m+1, k);
00080         t = -VAT(b, k);
00081         Vdaxpy(lm, t, RAT2(abd, la, k), 1, RAT(b, lb), 1);
00082     }
00083 }
00084
00085 VPUBLIC void Vdaxpy(int n, double da,
00086 double *dx, int incx,
00087 double *dy, int incy) {
00088
00089     int i, ix, iy, m, mpl;
00090
00091     if (n <= 0)
00092         return;
00093
00094     if (da == 0)
00095         return;
00096
00097     if (incx == 1 && incy == 1) {
00098
00099         m = n % 4;
00100         if (m != 0) {
00101
00102             for (i=1; i<=m; i++)
00103                 VAT(dy, i) += da * VAT(dx, i);
00104         }
00105
00106         if (n < 4)
00107             return;
00108
00109         mpl = m + 1;
00110
00111         for (i=mpl; i<=n; i+=4) {

```

```

00112
00113     VAT(dy, i ) += da * VAT(dx, i );
00114     VAT(dy, i+1) += da * VAT(dx, i+1);
00115     VAT(dy, i+2) += da * VAT(dx, i+2);
00116     VAT(dy, i+3) += da * VAT(dx, i+3);
00117 }
00118 } else {
00119
00120     ix = 1;
00121     if (incx < 0 )
00122         ix = (-n + 1) * incx + 1;
00123
00124     iy = 1;
00125     if (incy < 0 )
00126         iy = (-n + 1) * incy + 1;
00127
00128     for (i=1; i<=n; i++) {
00129
00130         VAT(dy, iy) += da * VAT(dx, ix);
00131         ix += incx;
00132         iy += incy;
00133     }
00134 }
00135 }
00136
00137
00138 VPUBLIC double Vddot(int n, double *dx, int incx, double *dy, int incy) {
00139
00140     double dtemp;
00141     int i, ix, iy, m, mpl;
00142
00143     double ddot = 0.0;
00144     dtemp = 0.0;
00145
00146     if (n <= 0)
00147         return ddot;
00148
00149     if (incx == 1 && incy == 1) {
00150
00151         m = n % 5;
00152
00153         if (m != 0) {
00154
00155             for (i=1; i<=m; i++)
00156                 dtemp += VAT(dx, i) * VAT(dy, i);
00157
00158             if (n < 5) {
00159                 ddot = dtemp;
00160                 return ddot;
00161             }
00162         }
00163
00164         mpl = m + 1;
00165
00166         for (i=mpl; i<=n; i+=5)
00167             dtemp += VAT(dx, i) * VAT(dy, i)
00168                 + VAT(dx, i+1) * VAT(dy, i+1)
00169                 + VAT(dx, i+2) * VAT(dy, i+2)
00170                 + VAT(dx, i+3) * VAT(dy, i+3)
00171                 + VAT(dx, i+4) * VAT(dy, i+4);
00172     } else {
00173
00174         ix = 1;
00175         if (incx < 0)
00176             ix = (-n + 1) * incx + 1;
00177
00178         iy = 1;
00179         if (incy < 0)
00180             iy = (-n + 1) * incy + 1;
00181
00182         for (i=1; i<=n; i++) {
00183             ix += incx;
00184             iy += incy;
00185         }
00186     }
00187
00188     ddot = dtemp;
00189     return ddot;
00190 }
00191
00192

```

```

00193
00194 VPUBLIC void Vdpbfa(double *abd, int *lda, int *n, int *m, int *info) {
00195
00196     double t, s;
00197     int ik, j, jk, k, mu;
00198
00199     MAT2(abd, *lda, 1);
00200
00201     *info = 0;
00202
00203     for(j = 1; j <= *n; j++) {
00204
00205         s = 0.0;
00206         ik = *m + 1;
00207         jk = VMAX2(j - *m, 1);
00208         mu = VMAX2(*m + 2 - j, 1);
00209
00210         if (*m >= mu ) {
00211
00212             for(k = mu; k <= *m; k++) {
00213                 t = VAT2(abd, k, j) - Vddot(k - mu,
00214                     RAT2(abd, ik, jk), 1,
00215                     RAT2(abd, mu, j), 1);
00216                 t /= VAT2(abd, *m + 1, jk);
00217                 VAT2(abd, k, j) = t;
00218                 s += t * t;
00219                 ik--;
00220                 jk++;
00221             }
00222         }
00223
00224         s = VAT2(abd, *m + 1, j) - s;
00225
00226         if (s <= 0.0) {
00227             *info = j;
00228             break;
00229         }
00230
00231         VAT2(abd, *m + 1, j) = VSQRT(s);
00232     }
00233 }

```

9.139 mlinpckd.h

```

00001
00049 #ifndef MLINPCKD_H_
00050 #define MLINPCKD_H_
00051
00052 #include "apbscfg.h"
00053
00054 #include "malloc/malloc.h"
00055
00056 #include "generic/vhal.h"
00057 #include "generic/vmatrix.h"
00058
00069 VEXTERNC void Vdpbsl(
00070     double *abd,
00071     int *lda,
00072     int *n,
00073     int *m,
00074     double *b
00075 );
00076
00080 VEXTERNC void Vdaxpy(int n, double da,
00081     double *dx, int incx,
00082     double *dy, int incy);
00083
00087 VEXTERNC double Vddot(int n, double *dx, int incx, double *dy, int incy);
00088
00092 VEXTERNC void Vdpbfa(double *abd, int *lda, int *n, int *m, int *info);
00093
00094 #endif /* MLINPCKD_H_ */

```

9.140 mypdec.c

```

00001

```

```

00055 #include "mypdec.h"
00056
00057 VPUBLIC void Vmypdefinitlpbe(int *tnion, double *tcharge, double *tsconc) {
00058     int i;
00059
00060     nion = *tnion;
00061     if (nion > MAXIONS) {
00062         Vnm_print(2, "Vmypde: Warning: Ignoring extra ion species\n");
00063         nion = MAXIONS;
00064     }
00065
00066     for (i=1; i<=nion; i++) {
00067         VAT(charge, i) = VAT(tcharge, i);
00068         VAT(sconc, i) = VAT(tsconc, i);
00069     }
00070 }
00071 }
00072
00073
00074
00075 VPUBLIC void Vmypdefinitnpbe(int *tnion, double *tcharge, double *tsconc) {
00076     int i;
00077
00078     nion = *tnion;
00079     if (nion > MAXIONS) {
00080         Vnm_print(2, "Vmypde: Warning: Ignoring extra ion species\n");
00081         nion = MAXIONS;
00082     }
00083
00084     for (i=1; i<=nion; i++) {
00085         VAT(charge, i) = VAT(tcharge, i);
00086         VAT(sconc, i) = VAT(tsconc, i);
00087     }
00088 }
00089 }
00090
00091
00092
00093 VPUBLIC void Vmypdefinitmpbe(int *tnion, double *tcharge, double *tsconc,
00094     double *smvolume, double *smsize) {
00095     int i;
00096
00097     WARN_UNTESTED;
00098
00099     VABORT_MSG0("Not tested");
00100
00101     if (*tnion > 3) {
00102         Vnm_print(2, "SMPBE: modified theory handles only three ion species.\n");
00103         Vnm_print(2, "      Ignoring the rest of the ions!\n");
00104         Vnm_print(2, "      (mypde.f::mypdefinit)\n");
00105     }
00106
00107     v1 = VAT(tcharge, 1);
00108     v2 = VAT(tcharge, 2);
00109     v3 = VAT(tcharge, 3);
00110     conc1 = VAT(tsconc, 1);
00111     conc2 = VAT(tsconc, 2);
00112     conc3 = VAT(tsconc, 3);
00113
00114     vol = *smvolume;
00115     relSize = *smsize;
00116 }
00117 }
00118
00119
00120
00121 VPUBLIC void Vc_vec(double *coef, double *uin, double *uout,
00122     int *nx, int *ny, int *nz, int *ipkey) {
00123
00124     if (*ipkey == -2) {
00125         Vc_vecsmpbe(coef, uin, uout, nx, ny, nz, ipkey);
00126     } else {
00127         Vc_vecpmg(coef, uin, uout, nx, ny, nz, ipkey);
00128     }
00129 }
00130
00131
00132
00133 VPUBLIC void Vc_vecpmg(double *coef, double *uin, double *uout,
00134     int *nx, int *ny, int *nz, int *ipkey) {
00135

```

```

00136     double zcf2;
00137     double zu2;
00138     double am_zero;
00139     double am_neg;
00140     double am_pos;
00141     double argument;
00142     int ichopped;
00143     int ichopped_neg;
00144     int ichopped_pos;
00145     int iion;
00146
00147     int n, i;
00148
00149     n = *nx * *ny * *nz;
00150
00151     for (i=1; i<=n; i++) {
00152         VAT(uout, i) = 0;
00153     }
00154
00155     for (iion=1; iion<=nion; iion++) {
00156
00157         // Assemble the ion-specific coefficient
00158         zcf2 = -1.0 * VAT(sconc, iion) * VAT(charge, iion);
00159
00160         // Assemble the ion-specific potential value
00161         zu2 = -1.0 * VAT(charge, iion);
00162
00163         if (*ipkey == 0) {
00164             ichopped = 0;
00165
00166             #pragma omp parallel for \
00167             default(shared) \
00168             private(i, ichopped_neg, ichopped_pos, am_zero, am_neg, am_pos, argument) \
00169             reduction(+ : ichopped)
00170             for (i=1; i<=n; i++) {
00171
00172                 // am_zero is 0 if coef zero, and 1 if coef nonzero
00173                 am_zero = VMIN2(ZSMALL, VABS(zcf2 * VAT(coef, i))) * ZLARGE;
00174
00175                 // am_neg is chopped u if u negative, 0 if u positive
00176                 am_neg = VMAX2(VMIN2(zu2 * VAT(uin, i), 0.0), SINH_MIN);
00177
00178                 // am_neg is chopped u if u positive, 0 if u negative
00179                 am_pos = VMIN2(VMAX2(zu2 * VAT(uin, i), 0.0), SINH_MAX);
00180
00181                 // Finally determine the function value
00182                 argument = am_zero * (am_neg + am_pos);
00183
00184                 VAT(uout, i) = VAT(uout, i) + zcf2 * VAT(coef, i) * exp(argument);
00185
00186                 // Count chopped values
00187                 ichopped_neg = (int)(am_neg / SINH_MIN);
00188                 ichopped_pos = (int)(am_pos / SINH_MAX);
00189                 ichopped += (int)(floor(am_zero+0.5)) * (ichopped_neg + ichopped_pos);
00190             }
00191
00192             // Info
00193             if (ichopped > 0) {
00194                 Vnm_print(2, "Vc_vecpmg: trapped exp overflows: %d\n", ichopped);
00195             }
00196
00197         } else if (*ipkey > 1 && *ipkey % 2 == 1 && *ipkey <= MAXPOLY) {
00198
00199             // Polynomial requested
00200             Vnm_print(2, "Vc_vecpmg: POLYNOMIAL APPROXIMATION UNAVAILABLE\n");
00201             abort();
00202         } else {
00203
00204             // Return linear approximation !***
00205             Vnm_print(2, "Vc_vecpmg: LINEAR APPROXIMATION UNAVAILABLE\n");
00206             abort();
00207         }
00208     }
00209 }
00210
00211
00212
00213 VPUBLIC void Vc_vecsmpbe(double *coef, double *uin, double *uout,
00214     int *nx, int *ny, int *nz, int *ipkey) {
00215
00216     int ideg;

```



```

00217     double zcf2, zu2;
00218     double am_zero, am_neg, am_pos;
00219     double argument, poly, fact;
00220
00221     int ichopped, ichopped_neg, ichopped_pos;
00222     int ion;
00223     int n, i, ii, ipara, ivect;
00224
00225     int nproc = 1;
00226
00227     // Added by DG SMPBE variables and common blocks
00228     double fracOccA, fracOccB, fracOccC, phi, ionStr;
00229     double z1, z2, z3, ca, cb, cc, a, k;
00230     double a1_neg, a1_pos, a2_neg, a2_pos;
00231     double a3_neg, a3_pos, a1, a2, a3;
00232     double f, g, gpark, alpha;
00233
00234     WARN_UNTESTED;
00235
00236     Vnm_print(2, "Vc_vecsmpbe: v1      = %f\n", v1);
00237     Vnm_print(2, "Vc_vecsmpbe: v2      = %f\n", v2);
00238     Vnm_print(2, "Vc_vecsmpbe: v3      = %f\n", v3);
00239     Vnm_print(2, "Vc_vecsmpbe: conc1   = %f\n", conc1);
00240     Vnm_print(2, "Vc_vecsmpbe: conc2   = %f\n", conc2);
00241     Vnm_print(2, "Vc_vecsmpbe: conc3   = %f\n", conc3);
00242     Vnm_print(2, "Vc_vecsmpbe: vol    = %f\n", vol);
00243     Vnm_print(2, "Vc_vecsmpbe: relSize = %f\n", relSize);
00244
00245     Vnm_print(2, "Vc_vecsmpbe: nion    = %d\n", nion);
00246
00247     Vnm_print(2, "Vc_vecsmpbe: charge = [");
00248     for (i=1; i<=nion; i++)
00249         Vnm_print(2, "%f ", VAT(charge, i));
00250     Vnm_print(2, "]\n");
00251
00252     Vnm_print(2, "Vc_vecsmpbe: sconc   = [");
00253     for (i=1; i<=nion; i++)
00254         Vnm_print(2, "%f ", VAT(sconc, i));
00255     Vnm_print(2, "]\n");
00256
00257
00258
00259     // Find parallel loops (ipara), remainder (ivect)
00260     n = *nx * *ny * *nz;
00261     ipara = n / nproc;
00262     ivect = n % nproc;
00263
00264     for (i=1; i<=n; i++)
00265         VAT(uout, i) = 0;
00266
00267     // Initialize the chopped counter
00268     ichopped = 0;
00269
00270     z1 = v1;
00271     z2 = v2;
00272     z3 = v3;
00273     ca = conc1;
00274     cb = conc2;
00275     cc = conc3;
00276     a = vol;
00277     k = relSize;
00278
00279     if (k - 1 < ZSMALL)
00280         Vnm_print(2, "Vc_vecsmpbe: k=1, using special routine\n");
00281
00282     // Derived quantities
00283     fracOccA = Na * ca * VPOW(a, 3.0);
00284     fracOccB = Na * cb * VPOW(a, 3.0);
00285     fracOccC = Na * cc * VPOW(a, 3.0);
00286
00287     phi = (fracOccA / k) + fracOccB + fracOccC;
00288     alpha = (fracOccA / k) / (1 - phi);
00289     ionStr = 0.5 * (ca * VPOW(z1, 2.0) + cb * VPOW(z2, 2.0) + cc * VPOW(z3, 2.0));
00290
00291     for (i=1; i<=n; i++) {
00292
00293         am_zero = VMIN2(ZSMALL, VABS(VAT(coef, i))) * ZLARGE;
00294
00295         // Compute the arguments for exp(-z*u) term
00296         a1_neg = VMAX2(VMIN2(-1.0 * z1 * VAT(uin, i), 0.0), SINH_MIN);
00297         a1_pos = VMIN2(VMAX2(-1.0 * z1 * VAT(uin, i), 0.0), SINH_MAX);

```

```

00298
00299 // Compute the arguments for exp(-u) term
00300 a2_neg = VMAX2(VMIN2(-1.0 * z2 * VAT(uin, i), 0.0), SINH_MIN);
00301 a2_pos = VMIN2(VMAX2(-1.0 * z2 * VAT(uin, i), 0.0), SINH_MAX);
00302
00303 // Compute the arguments for exp(u) term
00304 a3_neg = VMAX2(VMIN2(-1.0 * z3 * VAT(uin, i), 0.0), SINH_MIN);
00305 a3_pos = VMIN2(VMAX2(-1.0 * z3 * VAT(uin, i), 0.0), SINH_MAX);
00306
00307 a1 = am_zero * (a1_neg + a1_pos);
00308 a2 = am_zero * (a2_neg + a2_pos);
00309 a3 = am_zero * (a3_neg + a3_pos);
00310
00311 gpark = (1 + alpha * exp(a1)) / (1 + alpha);
00312
00313 if (k - 1 < ZSMALL) {
00314     f = z1 * ca * exp(a1) + z2 * cb * exp(a2) + z3 * cc * exp(a3);
00315     g = 1 - phi + fracOccA * exp(a1)
00316         + fracOccB * exp(a2)
00317         + fracOccC * exp(a3);
00318 } else {
00319     f = z1 * ca * exp(a1) * VPOW(gpark, k-1)
00320         + z2 * cb * exp(a2)
00321         + z3 * cc * exp(a3);
00322     g = (1 - phi + fracOccA / k) * VPOW(gpark, k)
00323         + fracOccB * exp(a2)
00324         + fracOccC * exp(a3);
00325 }
00326
00327 VAT(uout, i) = -1.0 * VAT(coef, i) * (0.5 / ionStr) * (f / g);
00328
00329 // Count chopped values
00330 ichopped_neg = (int)((a1_neg + a2_neg+a3_neg) / SINH_MIN);
00331 ichopped_pos = (int)((a1_pos + a2_pos+a3_pos) / SINH_MAX);
00332 ichopped += (int)floor(am_zero+0.5) * (ichopped_neg + ichopped_pos);
00333 }
00334
00335 // Info
00336 if (ichopped > 0)
00337     Vnm_print(2, "Vc_vecsmpbe: trapped exp overflows: %d\n", ichopped);
00338
00339 }
00340
00341 VPUBLIC void Vdc_vec(double *coef, double *uin, double *uout,
00342 int *nx, int *ny, int *nz, int *ipkey) {
00343
00344     int i;
00345     int n = *nx * *ny * *nz;
00346
00347     if(*ipkey == -2) {
00348         Vdc_vecsmpbe(coef, uin, uout, nx, ny, nz, ipkey);
00349     } else {
00350         Vdc_vecpmg(coef, uin, uout, nx, ny, nz, ipkey);
00351     }
00352 }
00353
00354 VPUBLIC void Vdc_vecpmg(double *coef, double *uin, double *uout,
00355 int *nx, int *ny, int *nz, int *ipkey) {
00356
00357     int ideg, iion;
00358     double zcf2, zu2;
00359     double am_zero, am_neg, am_pos;
00360     double argument, poly, fact;
00361
00362     int ichopped, ichopped_neg, ichopped_pos;
00363     int n, i;
00364
00365     // Find parallel loops (ipara), remainder (ivect)
00366     n = *nx * *ny * *nz;
00367
00368     for (i=1; i<=n; i++) {
00369         VAT(uout, i) = 0.0;
00370     }
00371
00372     for (iion=1; iion<=nion; iion++) {
00373
00374         zcf2 = VAT(sconc, iion) * VAT(charge, iion) * VAT(charge, iion);
00375         zu2 = -1.0 * VAT(charge, iion);
00376
00377         // Check if full exp requested
00378         if (*ipkey == 0) {

```

```

00379
00380 // Initialize chopped counter
00381 ichopped = 0;
00382
00383 #pragma omp parallel for \
00384 default(shared) \
00385 private(i, ichopped_neg, ichopped_pos, \
00386 am_zero, am_neg, am_pos, argument) \
00387 reduction(+:ichopped)
00388 for (i=1; i<=n; i++) {
00389
00390 // am_zero is 0 if coef zero, and 1 if coef nonzero
00391 am_zero = VMIN2(ZSMALL, VABS(zcf2 * VAT(coef, i))) * ZLARGE;
00392
00393 // am_neg is chopped u if u negative, 0 if u positive
00394 am_neg = VMAX2(VMIN2(zu2 * VAT(uin, i), 0.0), SINH_MIN);
00395
00396 // am_pos is chopped u if u positive, 0 if u negative
00397 am_pos = VMIN2(VMAX2(zu2 * VAT(uin, i), 0.0), SINH_MAX);
00398
00399 // Finally determine the function value
00400 argument = am_zero * (am_neg + am_pos);
00401 VAT(uout, i) += zcf2 * VAT(coef, i) * exp( argument );
00402
00403 // Count chopped values
00404 ichopped_neg = (int)(am_neg / SINH_MIN);
00405 ichopped_pos = (int)(am_pos / SINH_MAX);
00406 ichopped += (int)floor(am_zero+0.5) * (ichopped_neg + ichopped_pos);
00407 }
00408
00409 // Info
00410 if (ichopped > 0)
00411 Vnm_print(2, "Vdc_vec: trapped exp overflows: %d\n", ichopped);
00412
00413 } else if ((*ipkey) > 1 && (*ipkey) % 2 == 1 && (*ipkey) <= MAXPOLY) {
00414 VABORT_MSG0("Vdc_vec: Polynomial approximation unavailable\n");
00415 } else {
00416 VABORT_MSG0("Vdc_vec: Linear approximation unavailable\n");
00417 }
00418 }
00419 }
00420
00421
00422
00423 VPUBLIC void Vdc_vecsmpbe(double *coef, double *uin, double *uout,
00424 int *nx, int *ny, int *nz, int *ipkey) {
00425
00426 int ideg, ion;
00427 double zcf2, zu2;
00428 double am_zero, am_neg, am_pos;
00429 double argument, poly, fact;
00430 int ichopped, ichopped_neg, ichopped_pos;
00431
00432 int n, i, ii;
00433 int ipara, ivect;
00434
00435 int nproc = 1;
00436
00437 // Added by DG SMPBE variables and common blocks
00438 double fracOccA, fracOccB, fracOccC, phi, ionStr;
00439 double z1, z2, z3, ca, cb, cc, a, k;
00440 double a1_neg, a1_pos, a2_neg, a2_pos;
00441 double a3_neg, a3_pos, a1, a2, a3;
00442 double f, g, fprime, gprime, gpark, alpha;
00443
00444 WARN_UNTESTED;
00445
00446 // Find parallel loops (ipara), remainder (ivect)
00447 n = *nx * *ny * *nz;
00448 ipara = n / nproc;
00449 ivect = n % nproc;
00450
00451 for (i=1; i<=n; i++)
00452 VAT(uout, i) = 0.0;
00453
00454 // Initialize the chopped counter
00455 ichopped = 0;
00456
00457 z1 = v1;
00458 z2 = v2;
00459 z3 = v3;

```

```

00460     ca = conc1;
00461     cb = conc2;
00462     cc = conc3;
00463     a  = vol;
00464     k  = relSize;
00465
00466     if (k - 1 < ZSMALL)
00467         Vnm_print(2, "Vdc_vecsmpbe: k=1, using special routine\n");
00468
00469     // Derived quantities
00470     fracOccA = Na * ca * VPOW(a, 3.0);
00471     fracOccB = Na * cb * VPOW(a, 3.0);
00472     fracOccC = Na * cc * VPOW(a, 3.0);
00473     phi = fracOccA / k + fracOccB + fracOccC;
00474     alpha = (fracOccA / k) / (1 - phi);
00475     ionStr = 0.5*(ca * VPOW(z1, 2) + cb * VPOW(z2, 2) + cc * VPOW(z3, 2));
00476
00477     for (i=1; i<=n; i++) {
00478
00479         am_zero = VMIN2(ZSMALL, VABS(VAT(coef, i))) * ZLARGE;
00480
00481         // Compute the arguments for exp(-z*u) term
00482         a1_neg = VMAX2(VMIN2(-1.0 * z1 * VAT(uin, i), 0.0), SINH_MIN);
00483         a1_pos = VMIN2(VMAX2(-1.0 * z1 * VAT(uin, i), 0.0), SINH_MAX);
00484
00485         // Compute the arguments for exp(-u) term
00486         a2_neg = VMAX2(VMIN2(-1.0 * z2 * VAT(uin, i), 0.0), SINH_MIN);
00487         a2_pos = VMIN2(VMAX2(-1.0 * z2 * VAT(uin, i), 0.0), SINH_MAX);
00488
00489         // Compute the arguments for exp(u) term
00490         a3_neg = VMAX2(VMIN2(-1.0 * z3 * VAT(uin, i), 0.0), SINH_MIN);
00491         a3_pos = VMIN2(VMAX2(-1.0 * z3 * VAT(uin, i), 0.0), SINH_MAX);
00492
00493         a1 = am_zero * (a1_neg + a1_pos);
00494         a2 = am_zero * (a2_neg + a2_pos);
00495         a3 = am_zero * (a3_neg + a3_pos);
00496
00497         gpark = (1 + alpha * exp(a1)) / (1 + alpha);
00498
00499         if (k - 1 < ZSMALL) {
00500             f = z1 * ca * exp(a1) + z2 * cb * exp(a2) + z3 * cc * exp(a3);
00501             g = 1 - phi + fracOccA * exp(a1)
00502                 + fracOccB * exp(a2)
00503                 + fracOccC * exp(a3);
00504
00505             fprime =
00506                 - VPOW(z1, 2) * ca * exp(a1)
00507                 - VPOW(z2, 2) * cb * exp(a2)
00508                 - VPOW(z3, 2) * cc * exp(a3);
00509
00510             gprime =
00511                 - z1 * fracOccA * exp(a1)
00512                 - z2 * fracOccB * exp(a2)
00513                 - z3 * fracOccC * exp(a3);
00514         } else {
00515             f = z1 * ca * exp(a1) * VPOW(gpark, k - 1)
00516                 + z2 * cb * exp(a2)
00517                 + z3 * cc * exp(a3);
00518             g = (1 - phi + fracOccA / k) * VPOW(gpark, k)
00519                 + fracOccB * exp(a2)
00520                 + fracOccC * exp(a3);
00521
00522             fprime =
00523                 - VPOW(z1, 2) * ca * exp(a1) * VPOW(gpark, k - 2)
00524                 * (gpark + (k - 1) * (alpha / (1 + alpha)) * exp(a1))
00525                 - VPOW(z2, 2) * cb * exp(a2)
00526                 - VPOW(z3, 2) * cc * exp(a3);
00527
00528             gprime =
00529                 - k * z1 * (alpha / (1 + alpha)) * exp(a1)
00530                 * (1 - phi + fracOccA / k) * VPOW(gpark, k - 1)
00531                 - z2 * fracOccB * exp(a2)
00532                 - z3 * fracOccC * exp(a3);
00533         }
00534
00535         VAT(uout, i) = -1.0 * VAT(coef, i) * (0.5 / ionStr)
00536             * (fprime * g - gprime * f) / VPOW(g, 2.0);
00537
00538         // Count chopped values
00539         ichopped_neg = (int)((a1_neg + a2_neg + a3_neg) / SINH_MIN);
00540

```

```

00541         ichopped_pos = (int)((a1_pos + a2_pos + a3_pos) / SINH_MAX);
00542         ichopped += (int)floor(am_zero+0.5) * (ichopped_neg + ichopped_pos);
00543     }
00544
00545     // Info
00546     if (ichopped > 0)
00547         Vnm_print(2, "Vdc_vecsmpbe: trapped exp overflows: %d\n", ichopped);
00548 }

```

9.141 mypdec.h

```

00001
00050 #ifndef _MYPDE_H_
00051 #define _MYPDE_H_
00052
00053 #include "math.h"
00054
00055 #include "apbscfg.h"
00056
00057 #include "malloc/malloc.h"
00058
00059 #include "generic/vhal.h"
00060 #include "pmgc/mypdec.h"
00061
00062 #define MAXIONS    50
00063 #define MAXPOLY    50
00064 #define ZSMALL     1.0e-20
00065 #define ZLARGE     1.0e20
00066 #define SINH_MIN   -85.0
00067 #define SINH_MAX   85.0
00068
00070 double v1, v2, v3, conc1, conc2, conc3, vol, relSize;
00071 int nion;
00072 double charge[MAXIONS];
00073 double sconc[MAXIONS];
00074
00075 #define Na 6.022045000e-04
00076
00084 VEXTERNC void Vmypdefinitlpbe(
00085     int *tnion,
00086     double *tcharge,
00087     double *tsconc
00091 );
00092
00093
00094
00102 VEXTERNC void Vmypdefinitnpbe(
00103     int *tnion,
00104     double *tcharge,
00105     double *tsconc
00109 );
00110
00111
00112
00120 VEXTERNC void Vmypdefinitmpbe(
00121     int *tnion,
00122     double *tcharge,
00123     double *tsconc,
00127     double *smvolume,
00128     double *smsize
00129 );
00130
00131
00132
00139 VEXTERNC void Vc_vec(
00140     double *coef,
00141     double *uin,
00142     double *uout,
00143     int *nx,
00144     int *ny,
00145     int *nz,
00146     int *ipkey
00147 );
00148
00149
00150
00157 VEXTERNC void Vdc_vec(
00158     double *coef,

```

```

00159         double *uin,
00160         double *uout,
00161         int      *nx,
00162         int      *ny,
00163         int      *nz,
00164         int      *ipkey
00165     );
00166
00167 VEXTERNC void Vdc_vecpmg(
00168     double *coef,
00169     double *uin,
00170     double *uout,
00171     int     *nx,
00172     int     *ny,
00173     int     *nz,
00174     int     *ipkey
00175 );
00176
00177 VEXTERNC void Vdc_vecsmpbe(
00178     double *coef,
00179     double *uin,
00180     double *uout,
00181     int     *nx,
00182     int     *ny,
00183     int     *nz,
00184     int     *ipkey
00185 );
00186
00187
00188
00195 VEXTERNC void Vc_vecpmg(
00196     double *coef,
00197     double *uin,
00198     double *uout,
00199     int     *nx,
00200     int     *ny,
00201     int     *nz,
00202     int     *ipkey
00203 );
00204
00205
00206
00213 VEXTERNC void Vc_vecsmpbe(
00214     double *coef,
00215     double *uin,
00216     double *uout,
00217     int     *nx,
00218     int     *ny,
00219     int     *nz,
00220     int     *ipkey
00221 );
00222
00223 #endif /* _MYPDE_H_ */

```

9.142 newdrvd.c

```

00001
00055 #include "newdrvd.h"
00056
00057 VEXTERNC void Vnewdriv(
00058     int *iparm, double *rparm,
00059     int *iwork, double *rwork,
00060     double *u,
00061     double *xf, double *yf, double *zf,
00062     double *gxcf, double *gycf, double *gzcf,
00063     double *alcf, double *a2cf, double *a3cf,
00064     double *ccf, double *fcf, double *tcf) {
00065
00066     int nxc;
00067     int nyc;
00068     int nzc;
00069     int nf;
00070     int nc;
00071     int narr;
00072     int narrc;
00073     int n_rpc;
00074     int n_iz;
00075     int n_ipc;

```

```

00076     int iretot;
00077     int iintot;
00078
00079     int nrwk;
00080     int niwk;
00081     int nx;
00082     int ny;
00083     int nz;
00084     int nlev;
00085     int ierror;
00086     int maxlev;
00087     int mxlv;
00088     int mgcoar;
00089     int mgdisc;
00090     int mgsolv;
00091     int k_iz;
00092     int k_w1;
00093     int k_w2;
00094     int k_ipc;
00095     int k_rpc;
00096     int k_ac;
00097     int k_cc;
00098     int k_fc;
00099     int k_pc;
00100
00101     // Decode some parameters
00102     nrwk = VAT(iparm, 1);
00103     niwk = VAT(iparm, 2);
00104     nx = VAT(iparm, 3);
00105     ny = VAT(iparm, 4);
00106     nz = VAT(iparm, 5);
00107     nlev = VAT(iparm, 6);
00108
00109     // Some checks on input ***
00110     VASSERT_MSG0(nlev > 0, "The nlev parameter must be positive");
00111     VASSERT_MSG0(nx > 0, "The nx parameter must be positive");
00112     VASSERT_MSG0(ny > 0, "The ny parameter must be positive");
00113     VASSERT_MSG0(nz > 0, "The nz parameter must be positive");
00114
00115     mxlv = Vmaxlev(nx,ny,nz);
00116
00117     VASSERT_MSG1(nlev <= mxlv, "Max lev for your grid size is: %d", mxlv);
00118
00119     // Basic grid sizes, etc.
00120     mgcoar = VAT(iparm, 18);
00121     mgdisc = VAT(iparm, 19);
00122     mgsolv = VAT(iparm, 21);
00123
00124     Vmgsz(&mgcoar, &mgdisc, &mgsolv,
00125          &nx, &ny, &nz,
00126          &nlev,
00127          &nxc, &nyc, &nzc,
00128          &nf, &nc,
00129          &narr, &narrc,
00130          &n_rpc, &n_iz, &n_ipc,
00131          &iretot, &iintot);
00132
00133     // Allocate space for two additional work vectors ***
00134     iretot = iretot + 2 * nf;
00135
00136     // Some more checks on input
00137     VASSERT_MSG1(nrwk >= iretot, "Real work space must be: %d", iretot);
00138     VASSERT_MSG1(niwk >= iintot, "Integer work space must be: %d", iintot);
00139
00140     // Split up the integer work array
00141     k_iz = 1;
00142     k_ipc = k_iz + n_iz;
00143
00144     // Split up the real work array
00145     k_rpc = 1;
00146     k_cc = k_rpc + n_rpc;
00147     k_fc = k_cc + narr;
00148     k_w1 = k_fc + narr;
00149     k_w2 = k_w1 + nf;
00150     k_pc = k_w2 + nf;
00151     k_ac = k_pc + 27 * narrc;
00152     // k_ac_after = 4*nf + 14*narrc;
00153
00154     // Call the Newton Driver
00155     Vnewdrv2(iparm, rparm,
00156             &nx, &ny, &nz,

```

```

00157         u, RAT(iwork, k_iz),
00158         RAT(rwork, k_w1), RAT(rwork, k_w2),
00159         RAT(iwork, k_ipc), RAT(rwork, k_rpc),
00160         RAT(rwork, k_pc), RAT(rwork, k_ac), RAT(rwork, k_cc), RAT(rwork, k_fc),
00161         xf, yf, zf,
00162         gxcf, gycf, gzcf,
00163         alcf, a2cf, a3cf,
00164         ccfc, fcf, tcf);
00165     }
00166
00167
00168
00169 VPUBLIC void Vnewdriv2(int *iparm, double *rparm,
00170     int *nx, int *ny, int *nz,
00171     double *u, int *iz,
00172     double *w1, double *w2,
00173     int *ipc, double *rpc,
00174     double *pc, double *ac, double *cc, double *fc,
00175     double *xf, double *yf, double *zf,
00176     double *gxcf, double *gycf, double *gzcf,
00177     double *alcf, double *a2cf, double *a3cf,
00178     double *ccf, double *fcf, double *tcf) {
00179
00180     int mgkey;
00181     int nlev;
00182     int itmax;
00183     int iok;
00184     int iinfo;
00185     int istop;
00186     int ipkey;
00187     int nul;
00188     int nu2;
00189     int ilev;
00190     int ido;
00191     int iters;
00192     int ierror;
00193     int nlev_real;
00194     int ibound;
00195     int mgprol;
00196     int mgcoar;
00197     int mgsolv;
00198     int mgdisc;
00199     int mgsmoo;
00200     int mode;
00201     double epsiln;
00202     double epsmac;
00203     double errtol;
00204     double omegal;
00205     double omegan;
00206     double bf;
00207     double oh;
00208     double tsetupf;
00209     double tsetupc;
00210     double tsolve;
00211
00212
00213
00214     // Utility variables
00215     int numlev;
00216
00217     int iok_t;
00218     int iters_t;
00219     double rsnrm_t;
00220     double rsden_t;
00221     double orsnrm_t;
00222
00223     int i;
00224
00225
00226
00227     // Decode the iparm array
00228     nlev = VAT(iparm, 6);
00229     nul = VAT(iparm, 7);
00230     nu2 = VAT(iparm, 8);
00231     mgkey = VAT(iparm, 9);
00232     itmax = VAT(iparm, 10);
00233     istop = VAT(iparm, 11);
00234     iinfo = VAT(iparm, 12);
00235     ipkey = VAT(iparm, 14);
00236     mgprol = VAT(iparm, 17);
00237     mgcoar = VAT(iparm, 18);

```



```

00238     mgdisc = VAT(iparm, 19);
00239     mgsmoo = VAT(iparm, 20);
00240     mgsolv = VAT(iparm, 21);
00241
00242     errtol = VAT(rparm, 1);
00243     omegal = VAT(rparm, 9);
00244     omegan = VAT(rparm, 10);
00245
00246     Vprtstp(0, -99, 0.0, 0.0, 0.0);
00247
00248     // Build the multigrid data structure in iz
00249     Vbuildstr(nx, ny, nz, &nlev, iz);
00250
00251     // Start the timer
00252     Vnm_tstart(30, "Vnewdrv2: fine problem setup");
00253
00254     // Build op and rhs on fine grid ***
00255     ido = 0;
00256     Vbuildops(nx, ny, nz,
00257              &nlev, &ipkey, &iinfo, &ido, iz,
00258              &mgsprol, &mgscoar, &mgsolv, &mgdisc,
00259              ipc, rpc,
00260              pc, ac, cc, fc,
00261              xf, yf, zf,
00262              gxcf, gycf, gzcf,
00263              alcf, a2cf, a3cf,
00264              ccf, fcf, tcf);
00265
00266     // Stop the timer
00267     Vnm_tstop(30, "Vnewdrv2: fine problem setup");
00268
00269     // Start the timer
00270     Vnm_tstart(30, "Vnewdrv2: coarse problem setup");
00271
00272     // Build op and rhs on all coarse grids
00273     ido = 1;
00274     Vbuildops(nx, ny, nz,
00275              &nlev, &ipkey, &iinfo, &ido, iz,
00276              &mgsprol, &mgscoar, &mgsolv, &mgdisc,
00277              ipc, rpc,
00278              pc, ac, cc, fc,
00279              xf, yf, zf,
00280              gxcf, gycf, gzcf,
00281              alcf, a2cf, a3cf,
00282              ccf, fcf, tcf);
00283
00284     // Stop the timer
00285     Vnm_tstop(30, "Vnewdrv2: coarse problem setup");
00286
00287
00288
00289     /* *****
00290     * *** this overwrites the rhs array provided by pde specification ***
00291     * ***** compute an algebraically produced rhs for the given tcf ***
00292     * ***** */
00293     mode = 1;
00294
00295     if (istop == 4 || istop == 5) {
00296         WARN_UNTESTED;
00297         Vbuildalg(nx, ny, nz,
00298                 &mode, &nlev, iz,
00299                 ipc, rpc, ac, cc, ccf, tcf, fc, fcf);
00300     }
00301
00302
00303
00304     // Determine machine epsilon
00305     epsiln = Vnm_epsmac();
00306
00307     // Impose zero dirichlet boundary conditions (now in source fcn)
00308     VfboundPMG00(nx, ny, nz, u);
00309
00310     // Start the timer
00311     Vnm_tstart(30, "Vnewdrv2: solve");
00312
00313     // Call specified multigrid method
00314     nlev_real = nlev;
00315     iok = 1;
00316     ilev = 1;
00317     if (mgkey == 0) {
00318         Vnewton(nx, ny, nz,

```

```

00319         u, iz,
00320         ccf, fcf, w1, w2,
00321         &istop, &itmax, &iters, &ierror,
00322         &nlev, &ilev, &nlev_real, &mgsolv,
00323         &iok, &iinfo,
00324         &epsiln, &errtol, &omegan,
00325         &nul, &nu2, &mgs moo,
00326         alcf, a2cf, a3cf,
00327         ipc, rpc,
00328         pc, ac, cc, fc, tcf);
00329     } else if (mgkey == 1) {
00330         Vfnwton(nx, ny, nz,
00331         u, iz, ccf, fcf, w1, w2,
00332         &istop, &itmax, &iters, &ierror,
00333         &nlev, &ilev, &nlev_real, &mgsolv,
00334         &iok, &iinfo,
00335         &epsiln, &errtol, &omegan,
00336         &nul, &nu2, &mgs moo,
00337         alcf, a2cf, a3cf,
00338         ipc, rpc,
00339         pc, ac, cc, fc, tcf);
00340     } else {
00341         VABORT_MSG1("Bad mgkey given: %d", mgkey);
00342     }
00343
00344     // Stop the timer
00345     Vnm_tstop(30, "Vnewdrv2: solve");
00346
00347     // Restore boundary conditions
00348     ibound = 1;
00349     VfboundPMG(&ibound, nx, ny, nz, u, gxcf, gycf, gzcf);
00350 }

```

9.143 newdrv.h

```

00001
00050 #ifndef _NEWDRV_H_
00051 #define _NEWDRV_H_
00052
00053 #include "apbscfg.h"
00054
00055 #include "malloc/malloc.h"
00056
00057 #include "generic/vhal.h"
00058 #include "pmgc/mgs subd.h"
00059 #include "pmgc/mikpckd.h"
00060 #include "pmgc/newtond.h"
00061 #include "pmgc/mgdrv.h"
00062
00069 VEXTERN void Vnewdrv(
00070     int *iparm,
00071     double *rparm,
00072     int *iwork,
00073     double *rwork,
00074     double *u,
00075     double *xf,
00076     double *yf,
00077     double *zf,
00078     double *gxcf,
00079     double *gycf,
00080     double *gzcf,
00081     double *alcf,
00082     double *a2cf,
00083     double *a3cf,
00084     double *ccf,
00085     double *fcf,
00086     double *tcf
00087 );
00088
00125 VEXTERN void Vnewdrv2(
00126     int *iparm,
00127     double *rparm,
00128     int *nx,
00129     int *ny,
00130     int *nz,
00131     double *u,
00132     int *iz,
00133     double *wl,

```

```

00134         double *w2,
00135         int      *ipc,
00136         double *rpc,
00137         double *pc,
00138         double *ac,
00139         double *cc,
00140         double *fc,
00141         double *xf,
00142         double *yf,
00143         double *zf,
00144         double *gxcf,
00145         double *gycf,
00146         double *gzcf,
00147         double *alcf,
00148         double *a2cf,
00149         double *a3cf,
00150         double *ccf,
00151         double *fcf,
00152         double *tcf
00153     );
00154
00155 #endif /* _NEWDRVD_H_ */

```

9.144 newtond.c

```

00001
00056 #include "newtond.h"
00057
00058 VPUBLIC void Vfnewton(int *nx,int *ny,int *nz,
00059     double *x, int *iz,
00060     double *w0, double *w1, double *w2, double *w3,
00061     int *istop, int *itmax, int *iters, int *ierror,
00062     int *nlev, int *ilev, int *nlev_real,
00063     int *mgsolv, int *iok, int *iinfo,
00064     double *epsiln, double *errtol, double *omega,
00065     int *nul, int *nu2, int *mgsmoo,
00066     double *cprime, double *rhs, double *xtmp,
00067     int *ipc, double *rpc,
00068     double *pc, double *ac, double *cc, double *fc, double *tru) {
00069
00070     int level, itmxd, nlevd, iterd, iokd;
00071     int nxf, nyf, nzf;
00072     int nxc, nyc, nzc;
00073     int istpd;
00074     int numlev;
00075     double errd;
00076
00077     MAT2( iz, 50, 1);
00078
00079     // Recover gridsizes ***
00080     nxf = *nx;
00081     nyf = *ny;
00082     nzf = *nz;
00083
00084     numlev = *nlev - 1;
00085     Vmkcors(&numlev, &nxf, &nyf, &nzf, &nxc, &nyc, &nzc);
00086
00087     // Move up grids: interpolate solution to finer, do newton
00088     if (*iinfo > 1) {
00089         VMESAGE0("Starting");
00090         VMESAGE3("Fine Grid Size:  (%d, %d, %d)", nxf, nyf, nzf);
00091         VMESAGE3("Course Grid Size: (%d, %d, %d)", nxc, nyc, nzc);
00092     }
00093
00094     for (level=*nlev_real; level<=*ilev+1; level--) {
00095
00096         // Call mv cycle
00097         errd = *errtol;
00098         itmxd = 1000;
00099         nlevd = *nlev_real - level + 1;
00100         iterd = 0;
00101         iokd = *iok;
00102         istpd = *istop;
00103
00104         Vnewton(&nxc, &nyc, &nzc,
00105             x, iz,
00106             w0, w1, w2, w3,
00107             &istpd, &itmxd, &iterd, ierror,

```

```

00108         &nlevd, &level, nlev_real,
00109         mgsolv, &iokd, iinfo,
00110         epsiln, &errd, omega,
00111         nul, nu2, mgsmoo,
00112         cprime, rhs, xtmp,
00113         ipc, rpc,
00114         pc, ac, cc, fc, tru);
00115
00116
00117         // Find new grid size ***
00118         numlev = 1;
00119         Vmkfine(&numlev, &nxc, &nyc, &nzc, &nxf, &nyf, &nzf);
00120
00121         // Interpolate to next finer grid (use correct bc's)
00122         VinterpPMG(&nxc, &nyc, &nzc,
00123                 &nxf, &nyf, &nzf,
00124                 RAT( x, VAT2(iz, 1, level )),
00125                 RAT( x, VAT2(iz, 1, level-1)),
00126                 RAT(pc, VAT2(iz, 11, level-1)));
00127
00128         /*
00129         Commented out fortran code. May need to implement later
00130         call ninterpPMG(nxc,nyc,nzc,nxf,nyf,nzf,
00131                 x(iz(1,level)),x(iz(1,level-1)),pc(iz(11,level-1)),
00132                 ipc(iz(5,level-1)),rpc(iz(6,level-1)),
00133                 ac(iz(7,level-1)),cc(iz(1,level-1)),fc(iz(1,level-1)))
00134         */
00135
00136         // New grid size
00137         nxc = nxf;
00138         nyc = nyf;
00139         nzc = nzf;
00140     }
00141
00142
00143
00144     // Call mv cycle
00145     level = *ilev;
00146
00147     Vnewton(nx, ny, nz,
00148             x, iz,
00149             w0, w1, w2, w3,
00150             istop, itmax, iters, ierror,
00151             nlev, &level, nlev_real,
00152             mgsolv, iok, iinfo,
00153             epsiln, errtol, omega,
00154             nul, nu2, mgsmoo,
00155             cprime, rhs, xtmp,
00156             ipc, rpc,
00157             pc, ac, cc, fc, tru);
00158 }
00159
00160
00161
00162 VPUBLIC void Vnewton(int *nx, int *ny, int *nz,
00163         double *x, int *iz,
00164         double *w0, double *w1, double *w2, double *w3,
00165         int *istop, int *itmax, int *iters, int *ierror,
00166         int *nlev, int *ilev, int *nlev_real,
00167         int *mgsolv, int *iok, int *iinfo,
00168         double *epsiln, double *errtol, double *omega,
00169         int *nul, int *nu2, int *mgsmoo,
00170         double *cprime, double *rhs, double *xtmp,
00171         int *ipc, double *rpc,
00172         double *pc, double *ac, double *cc, double *fc, double *tru) {
00173
00174     int level, lev;
00175     int itmax_s, iters_s, ierror_s, iok_s, iinfo_s, istop_s;
00176     double errtol_s, ord, bigc;
00177     double rsden, rsnm, orsnrm;
00178
00179     double xnorm_old, xnorm_new, damp, xnorm_med, xnorm_den;
00180     double rho_max, rho_min, rho_max_mod, rho_min_mod, errtol_p;
00181     int iter_d, itmax_d, mode, idamp, ipkey;
00182     int itmax_p, iters_p, iok_p, iinfo_p;
00183
00184     // Utility and temporary parameters
00185     double alpha;
00186
00187     MAT2(iz, 50, 1);
00188

```

```

00189 // Recover level information
00190 level = 1;
00191 lev = (*ilev - 1) + level;
00192
00193 // Do some i/o if requested
00194 if (*iinfo > 1) {
00195     VMESAGE3("Starting: (%d, %d, %d)", *nx, *ny, *nz);
00196 }
00197
00198 if (*iok != 0) {
00199     Vprtstp(*iok, -1, 0.0, 0.0, 0.0);
00200 }
00201
00202 /*****
00203 *** note: if (iok!=0) then: use a stopping test. ***
00204 *** else: use just the itmax to stop iteration. ***
00205 *****/
00206 *** istop=0 most efficient (whatever it is) ***
00207 *** istop=1 relative residual ***
00208 *** istop=2 rms difference of successive iterates ***
00209 *** istop=3 relative true error (provided for testing) ***
00210 *****/
00211
00212 // Compute denominator for stopping criterion
00213 if (*istop == 0) {
00214     rsden = 1.0;
00215 } else if (*istop == 1) {
00216     // Compute initial residual with zero initial guess
00217     // this is analogous to the linear case where one can
00218     // simply take norm of rhs for a zero initial guess
00219
00220     Vazeros(nx, ny, nz, w1);
00221
00222     Vnmresid(nx, ny, nz,
00223             RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00224             RAT(ac, VAT2(iz, 7, lev)), RAT(cc, VAT2(iz, 1, lev)),
00225             RAT(fc, VAT2(iz, 1, lev)),
00226             w1, w2, w3);
00227     rsden = Vxnrm1(nx, ny, nz, w2);
00228 } else if (*istop == 2) {
00229     rsden = VSQRT(*nx * *ny * *nz);
00230 } else if (*istop == 3) {
00231     rsden = Vxnrm2(nx, ny, nz, RAT(tru, VAT2(iz, 1, lev)));
00232 } else if (*istop == 4) {
00233     rsden = Vxnrm2(nx, ny, nz, RAT(tru, VAT2(iz, 1, lev)));
00234 } else if (*istop == 5) {
00235     Vnmatvec(nx, ny, nz,
00236             RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00237             RAT(ac, VAT2(iz, 7, lev)), RAT(cc, VAT2(iz, 1, lev)),
00238             RAT(tru, VAT2(iz, 1, lev)),
00239             w1, w2);
00240     rsden = VSQRT(Vxdot(nx, ny, nz, RAT(tru, VAT2(iz, 1, lev)), w1));
00241 } else {
00242     VABORT_MSG1("Bad istop value: %d\n", *istop);
00243 }
00244
00245 if (rsden == 0.0) {
00246     rsden = 1.0;
00247     VWARN_MSG0(rsden != 0, "rhs is zero");
00248 }
00249 rsnm = rsden;
00250 orsnrm = rsnm;
00251
00252 if (*iok != 0) {
00253     Vprtstp(*iok, 0, rsnm, rsden, orsnrm);
00254 }
00255
00256 /*****
00257 *** begin newton iteration
00258 *****/
00259
00260 // Now compute residual with the initial guess
00261
00262 Vnmresid(nx, ny, nz,
00263         RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00264         RAT(ac, VAT2(iz, 7, lev)), RAT(cc, VAT2(iz, 1, lev)),
00265         RAT(fc, VAT2(iz, 1, lev)), RAT(x, VAT2(iz, 1, lev)),
00266         w0, w2);
00267 xnorm_old = Vxnrm1(nx, ny, nz, w0);
00268 if (*iok != 0) {

```

```

00270         xnorm_den = rsden;
00271     } else {
00272         xnorm_den = xnorm_old;
00273     }
00274
00275
00276
00277     /*****
00278     *** begin the loop
00279     *****/
00280
00281     // Setup for the looping
00282     VMESAGE0("Damping enabled");
00283     idamp = 1;
00284     *iters = 0;
00285
00286     //30
00287     while(1) {
00288
00289         (*iters)++;
00290
00291         // Save iterate if stop test will use it on next iter
00292         if (*istop == 2) {
00293             Vxcopy(nx, ny, nz,
00294                 RAT(x, VAT2(iz, 1, lev)), RAT(tru, VAT2(iz, 1, lev)));
00295         }
00296
00297         // Compute the current jacobian system and rhs
00298         ipkey = VAT(ipc, 10);
00299         Vgetjac(nx, ny, nz, nlev_real, iz, ilev, &ipkey,
00300             x, w0, cprime, rhs, cc, pc);
00301
00302         // Determine number of correct digits in current residual
00303         // Algorithm 5.3 in the thesis, test version (1')
00304         // Global-superlinear convergence
00305         bigc = 1.0;
00306         ord = 2.0;
00307
00308         /* NAB 06-18-01: If complex problems are not converging, set this to
00309         * machine epsilon. This makes it use the exact jacobian rather than
00310         * the appropriate form (as here)
00311         */
00312         errtol_s = VMIN2((0.9 * xnorm_old), (bigc * VPOW(xnorm_old, ord)));
00313         VMESAGE1("Using errtol_s: %f", errtol_s);
00314
00315         // Do a linear multigrid solve of the newton equations
00316         Vazeros(nx, ny, nz, RAT(xtmp, VAT2(iz, 1, lev)));
00317
00318         itmax_s = 1000;
00319         istop_s = 0;
00320         iters_s = 0;
00321         ierror_s = 0;
00322
00323         // NAB 06-18-01 -- What this used to be:
00324         iok_s = 0;
00325         iinfo_s = 0;
00326         if ((*iinfo >= 2) && (*ilev == 1))
00327             iok_s = 2;
00328
00329         // What it's changed to:
00330         if (*iinfo >= 2)
00331             iinfo_s = *iinfo;
00332         iok_s = 2;
00333
00334         // End of NAB hack.
00335
00336         Vmvcs(nx, ny, nz,
00337             xtmp, iz,
00338             w0, w1, w2, w3,
00339             &istop_s, &itmax_s, &iters_s, &ierror_s,
00340             nlev, ilev, nlev_real, mgsolv,
00341             &iok_s, &iinfo_s,
00342             epsiln, &errtol_s, omega,
00343             nul, nu2, mgsmoo,
00344             ipc, rpc, pc, ac, cprime, rhs, tru);
00345
00346         /*****
00347         *** note: rhs and cprime are now available as temp vectors ***
00348         *****/
00349
00350         // If damping is still enabled -- doit

```

```

00351     if (idamp == 1) {
00352
00353         // Try the correction
00354         Vxcopy(nx, ny, nz,
00355              RAT(x, VAT2(iz, 1, lev)), w1);
00356         damp = 1.0;
00357         Vxaxpy(nx, ny, nz, &damp, RAT(xtmp, VAT2(iz, 1, lev)), w1);
00358
00359         Vnmresid(nx, ny, nz,
00360              RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00361              RAT(ac, VAT2(iz, 7, lev)), RAT(cc, VAT2(iz, 1, lev)),
00362              RAT(fc, VAT2(iz, 1, lev)),
00363              w1, w0,
00364              RAT(rhs, VAT2(iz, 1, lev)));
00365         xnorm_new = Vxnrm1(nx, ny, nz, w0);
00366
00367         // Damping is still enabled -- doit
00368         damp = 1.0;
00369         iter_d = 0;
00370         itmax_d = 10;
00371         mode = 0;
00372
00373         VMESAGE1("Attempting damping, relres = %f", xnorm_new / xnorm_den);
00374
00375         while(iter_d < itmax_d) {
00376             if (mode == 0) {
00377                 if (xnorm_new < xnorm_old) {
00378                     mode = 1;
00379                 }
00380             } else if (xnorm_new > xnorm_med) {
00381                 break;
00382             }
00383
00384             // Keep old soln and residual around, and its norm
00385             Vxcopy(nx, ny, nz, w1, w2);
00386             Vxcopy(nx, ny, nz, w0, w3);
00387             xnorm_med = xnorm_new;
00388
00389             // New damped correction, residual, and its norm
00390             Vxcopy(nx, ny, nz,
00391                  RAT(x, VAT2(iz, 1, lev)), w1);
00392             damp = damp / 2.0;
00393             Vxaxpy(nx, ny, nz, &damp, RAT(xtmp, VAT2(iz, 1, lev)), w1);
00394
00395             Vnmresid(nx, ny, nz,
00396                  RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00397                  RAT(ac, VAT2(iz, 7, lev)), RAT(cc, VAT2(iz, 1, lev)),
00398                  RAT(fc, VAT2(iz, 1, lev)),
00399                  w1, w0,
00400                  RAT(rhs, VAT2(iz, 1, lev)));
00401             xnorm_new = Vxnrm1(nx, ny, nz, w0);
00402
00403             // Next iter...
00404             iter_d = iter_d + 1;
00405             VMESAGE1("Attempting damping, relres = %f",
00406                  xnorm_new / xnorm_den);
00407
00408         }
00409
00410         Vxcopy(nx, ny, nz, w2, RAT(x, VAT2(iz, 1, lev)));
00411         Vxcopy(nx, ny, nz, w3, w0);
00412         xnorm_new = xnorm_med;
00413         xnorm_old = xnorm_new;
00414
00415         VMESAGE1("Damping accepted, relres = %f", xnorm_new / xnorm_den);
00416
00417         // Determine whether or not to disable damping
00418         if ((iter_d - 1) == 0) {
00419             VMESAGE0("Damping disabled");
00420             idamp = 0;
00421         }
00422     } else {
00423
00424         // Damping is disabled -- accept the newton step
00425         damp = 1.0;
00426
00427         Vxaxpy(nx, ny, nz, &damp,
00428              RAT(xtmp, VAT2(iz, 1, lev)), RAT(x, VAT2(iz, 1, lev)));
00429
00430         Vnmresid(nx, ny, nz,
00431              RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),

```

```

00432         RAT( ac, VAT2(iz, 7, lev)), RAT( cc, VAT2(iz, 1, lev)),
00433         RAT( fc, VAT2(iz, 1, lev)), RAT( x, VAT2(iz, 1, lev)),
00434         w0,
00435         RAT(rhs, VAT2(iz, 1, lev)));
00436
00437     xnorm_new = Vxnrm1(nx, ny, nz, w0);
00438     xnorm_old = xnorm_new;
00439 }
00440
00441 // Compute/check the current stopping test ***
00442 if (iok != 0) {
00443
00444     orsnrm = rsnm;
00445
00446     if (*istop == 0) {
00447         rsnm = xnorm_new;
00448     } else if (*istop == 1) {
00449         rsnm = xnorm_new;
00450     } else if (*istop == 2) {
00451         Vxcopy(nx, ny, nz, RAT(tru, VAT2(iz, 1, lev)), w1);
00452         alpha = -1.0;
00453         Vxaxpy(nx, ny, nz, &alpha, RAT(x, VAT2(iz, 1, lev)), w1);
00454         rsnm = Vxnrm1(nx, ny, nz, w1);
00455     } else if (*istop == 3) {
00456         Vxcopy(nx, ny, nz, RAT(tru, VAT2(iz, 1, lev)), w1);
00457         alpha = -1.0;
00458         Vxaxpy(nx, ny, nz, &alpha, RAT(x, VAT2(iz, 1, lev)), w1);
00459         rsnm = Vxnrm2(nx, ny, nz, w1);
00460     } else if (*istop == 4) {
00461         Vxcopy(nx, ny, nz, RAT(tru, VAT2(iz, 1, lev)), w1);
00462         alpha = -1.0;
00463         Vxaxpy(nx, ny, nz, &alpha, RAT(x, VAT2(iz, 1, lev)), w1);
00464         rsnm = Vxnrm2(nx, ny, nz, w1);
00465     } else if (*istop == 5) {
00466         Vxcopy(nx, ny, nz, RAT(tru, VAT2(iz, 1, lev)), w1);
00467         alpha = -1.0;
00468         Vxaxpy(nx, ny, nz, &alpha, RAT(x, VAT2(iz, 1, lev)), w1);
00469         Vnmatvec(nx, ny, nz,
00470                 RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00471                 RAT( ac, VAT2(iz, 7, lev)), RAT( cc, VAT2(iz, 1, lev)),
00472                 w1, w2, w3);
00473         rsnm = VSQRT(Vxdot(nx, ny, nz, w1, w2));
00474     } else {
00475         VABORT_MSG1("Bad istop value: %d", *istop);
00476     }
00477
00478     Vprtstp(*iok, *iters, rsnm, rsden, orsnrm);
00479
00480     if ((rsnm/rsden) <= *errtol)
00481         break;
00482 }
00483
00484 // Check iteration count ***
00485 if (*iters >= *itmax)
00486     break;
00487 }
00488
00489 // Condition estimate of final jacobian
00490 if (*iinfo > 2) {
00491
00492     Vnm_print(2, "%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%\n");
00493     Vnm_print(2, "% Vnewton: JACOBIAN ANALYSIS ==> (%d, %d, %d)\n",
00494             *nx, *ny, *nz );
00495
00496     // Largest eigenvalue of the jacobian matrix
00497     Vnm_print(2, "% Vnewton: Power calculating rho(JAC)\n");
00498     itmax_p = 1000;
00499     errtol_p = 1.0e-4;
00500     iters_p = 0;
00501     iinfo_p = *iinfo;
00502
00503     Vpower(nx, ny, nz,
00504           iz, ilev,
00505           ipc, rpc, ac, cprime,
00506           w0, w1, w2, w3,
00507           &rho_max, &rho_max_mod,
00508           &errtol_p, &itmax_p, &iters_p, &iinfo_p);
00509
00510     Vnm_print(2, "% Vnewton: power iters = %d\n", iters_p);
00511     Vnm_print(2, "% Vnewton: power eigmax = %d\n", rho_max);
00512     Vnm_print(2, "% Vnewton: power (MODEL) = %d\n", rho_max_mod);

```



```

00513
00514 // Smallest eigenvalue of the system matrix A ***
00515 Vnm_print(2, "% Vnewton: ipower calculating lambda_min(JAC)...\\n");
00516 itmax_p = 1000;
00517 errtol_p = 1.0e-4;
00518 iters_p = 0;
00519 iinfo_p = *iinfo;
00520
00521 Vazeros(nx, ny, nz, xtmp);
00522
00523 Vipower(nx, ny, nz,
00524         xtmp, iz,
00525         w0, w1, w2, w3,
00526         rhs, &rho_min, &rho_min_mod,
00527         &errtol_p, &itmax_p, &iters_p,
00528         nlev, ilev, nlev_real, mgsolv,
00529         &iok_p, &iinfo_p,
00530         epsiln, errtol, omega,
00531         nul, nu2, mgsmoo,
00532         ipc, rpc,
00533         pc, ac, cprime, tru);
00534
00535 Vnm_print(2, "% Vnewton: ipower iters = %d\\n", iters_p);
00536 Vnm_print(2, "% Vnewton: ipower eigmin = %d\\n", rho_min);
00537 Vnm_print(2, "% Vnewton: ipower (MODEL) = %d\\n", rho_min_mod);
00538
00539 // Condition number estimate
00540 Vnm_print(2, "% Vnewton: condition number = %f\\n",
00541         (double)rho_max / rho_min);
00542 Vnm_print(2, "% Vnewton: condition (MODEL) = %f\\n",
00543         (double)rho_max_mod / rho_min_mod);
00544 Vnm_print(2, "%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%\\n");
00545 }
00546 }
00547
00548
00549
00550 VPUBLIC void Vgetjac(int *nx, int *ny, int *nz,
00551                    int *nlev_real, int *iz, int *lev, int *ipkey,
00552                    double *x, double *r,
00553                    double *cprime, double *rhs,
00554                    double *cc, double *pc) {
00555
00556     int nxx, nyy, nzz;
00557     int nxold, nyold, nzold;
00558     int level, numlev;
00559
00560     MAT2(iz, 50, 1);
00561
00562     // Setup
00563     nxx = *nx;
00564     nyy = *ny;
00565     nzz = *nz;
00566
00567     // Form the rhs of the newton system -- just current residual
00568     Vxcopy(nx, ny, nz, r, RAT(rhs, VAT2(iz, 1,*lev)));
00569
00570     // Get nonlinear part of the jacobian operator
00571     Vdc_vec(RAT(cc, VAT2(iz, 1,*lev)), RAT(x, VAT2(iz, 1,*lev)),
00572            RAT(cprime, VAT2(iz, 1,*lev)),
00573            nx, ny, nz, ipkey);
00574
00575     // Build the (nlev-1) level operators
00576     for (level=*lev+1; level<=*nlev_real; level++) {
00577         nxold = nxx;
00578         nyold = nyy;
00579         nzold = nzz;
00580
00581         numlev = 1;
00582         Vmkcors(&numlev, &nxold, &nyold, &nzold, &nxx, &nyy, &nzz);
00583
00584         // Make the coarse grid rhs functions
00585         Vrestrc(&nxold, &nyold, &nzold,
00586                &nxx, &nyy, &nzz,
00587                RAT(rhs, VAT2(iz, 1,level-1)),
00588                RAT(rhs, VAT2(iz, 1,level )),
00589                RAT( pc, VAT2(iz, 1,level-1)));
00590
00591         // Make the coarse grid helmholtz terms
00592         Vrestrc(&nxold, &nyold, &nzold,
00593                &nxx, &nyy, &nzz,

```

```

00594         RAT(cprime, VAT2(iz, 1, level-1)),
00595         RAT(cprime, VAT2(iz, 1, level )),
00596         RAT(    pc, VAT2(iz, 11, level-1));
00597     }
00598 }

```

9.145 newtond.h

```

00001
00049 #ifndef _NEWTOND_H_
00050 #define _NEWTOND_H_
00051
00052 #include "apbscfg.h"
00053
00054 #include "malloc/malloc.h"
00055
00056 #include "generic/vhal.h"
00057 #include "generic/vmatrix.h"
00058 #include "pmgc/matvecd.h"
00059 #include "pmgc/mikpckd.h"
00060 #include "pmgc/mgcsd.h"
00061 #include "pmgc/mgsudd.h"
00062 #include "pmgc/powerd.h"
00063
00070 VPUBLIC void Vfnewton(
00071     int *nx,
00072     int *ny,
00073     int *nz,
00074     double *x,
00075     int *iz,
00076     double *w0,
00077     double *w1,
00078     double *w2,
00079     double *w3,
00080     int *istop,
00081     int *itmax,
00082     int *iters,
00083     int *ierror,
00084     int *nlev,
00085     int *ilev,
00086     int *nlev_real,
00087     int *mgsolv,
00088     int *iick,
00089     int *iinfo,
00090     double *epsiln,
00091     double *errtol,
00092     double *omega,
00093     int *nul,
00094     int *nu2,
00095     int *mgsmoo,
00096     double *cprime,
00097     double *rhs,
00098     double *xtmp,
00099     int *ipc,
00100     double *rpc,
00101     double *pc,
00102     double *ac,
00103     double *cc,
00104     double *fc,
00105     double *tru
00106 );
00107
00114 VEXTERNC void Vnewton(
00115     int *nx,
00116     int *ny,
00117     int *nz,
00118     double *x,
00119     int *iz,
00120     double *w0,
00121     double *w1,
00122     double *w2,
00123     double *w3,
00124     int *istop,
00125     int *itmax,
00126     int *iters,
00127     int *ierror,
00128     int *nlev,
00129     int *ilev,

```

```

00130         int *nlev_real,
00131         int *mgsolv,
00132         int *iok,
00133         int *iinfo,
00134         double *epsiln,
00135         double *errtol,
00136         double *omega,
00137         int *nu1,
00138         int *nu2,
00139         int *mgsmoo,
00140         double *cprime,
00141         double *rhs,
00142         double *xtmp,
00143         int *ipc,
00144         double *rpc,
00145         double *pc,
00146         double *ac,
00147         double *cc,
00148         double *fc,
00149         double *tru
00150     );
00151
00152
00159 VEXTERNC void Vgetjac(
00160     int *nx,
00161     int *ny,
00162     int *nz,
00163     int *nlev_real,
00164     int *iz,
00165     int *lev,
00166     int *ipkey,
00167     double *x,
00168     double *r,
00169     double *cprime,
00170     double *rhs,
00171     double *cc,
00172     double *pc
00173 );
00174
00175 #endif /* _NEWTOND_H_ */

```

9.146 powerd.c

```

00001
00055 #include "powerd.h"
00056
00057 VPUBLIC void Vpower(int *nx, int *ny, int *nz,
00058     int *iz, int *ilev,
00059     int *ipc, double *rpc, double *ac, double *cc,
00060     double *w1, double *w2, double *w3, double *w4,
00061     double *eigmax, double *eigmax_model, double *tol,
00062     int *itmax, int *iters, int *iinfo) {
00063
00064     int lev, level;
00065     double denom, fac, rho, oldrho, error, relerr;
00066
00068     double pi = 4.0 * atan( 1.0 );
00069
00070     // Utility variables
00071     int skipIters = 0;
00072     double alpha;
00073
00074     MAT2(iz, 50, 1);
00075
00076     WARN_UNTESTED;
00077
00078     // Recover level information
00079     level = 1;
00080     lev = (*ilev - 1) + level;
00081
00082     // Seed vector: random to contain all components
00083
00084     Vaxrand(nx, ny, nz, w1);
00085
00086     Vazeros(nx, ny, nz, w2);
00087     Vazeros(nx, ny, nz, w3);
00088     Vazeros(nx, ny, nz, w4);
00089

```

```

00090 // Compute raleigh quotient with the seed vector
00091 denom = Vxnorm2(nx, ny, nz, w1);
00092 fac = 1.0 / denom;
00093 Vxscal(nx, ny, nz, &fac, w1);
00094 Vmatvec(nx, ny, nz,
00095         RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00096         RAT(ac, VAT2(iz, 7, lev)), RAT(cc, VAT2(iz, 1, lev)), w1, w2);
00097 oldrho = Vxdot(nx, ny, nz, w1, w2);
00098
00099 // I/O
00100 if (oldrho == 0.0) {
00101     if (*iinfo > 3) {
00102         Vnm_print(2, "POWER: iter: estimate = %d %g\n", *iters, oldrho);
00103     }
00104     rho = oldrho;
00105 } else {
00106
00107     // Main iteration
00108     *iters = 0;
00109     while(1) {
00110         (*iters)++;
00111
00112         // Apply the matrix A
00113         Vmatvec(nx, ny, nz,
00114                 RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00115                 RAT(ac, VAT2(iz, 7, lev)), RAT(cc, VAT2(iz, 1, lev)), w1, w2);
00116
00117         Vxcopy(nx, ny, nz, w2, w1);
00118
00119         // Normalize the new vector
00120         denom = Vxnorm2(nx, ny, nz, w1);
00121         fac = 1.0 / denom;
00122         Vxscal(nx, ny, nz, &fac, w1);
00123
00124         // Compute the new raleigh quotient
00125         Vmatvec(nx, ny, nz,
00126                 RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00127                 RAT(ac, VAT2(iz, 7, lev)), RAT(cc, VAT2(iz, 1, lev)), w1, w2);
00128         rho = Vxdot(nx, ny, nz, w1, w2);
00129
00130         // Stopping test ***
00131         // w2=A*x, w1=x, stop = 2-norm(A*x-lamda*x)
00132
00133         Vxcopy(nx, ny, nz, w1, w3);
00134         Vxcopy(nx, ny, nz, w2, w4);
00135         Vxscal(nx, ny, nz, &rho, w3);
00136         alpha = -1.0;
00137         Vxaxpy(nx, ny, nz, &alpha, w3, w4);
00138         error = Vxnorm2(nx, ny, nz, w4);
00139         relerr = VABS(rho - oldrho) / VABS(rho);
00140
00141         // I/O
00142         if (*iinfo > 3) {
00143
00144             Vnm_print(2, "POWER:  iters  =%d\n", *iters);
00145             Vnm_print(2, "          error  =%g\n", error);
00146             Vnm_print(2, "          relerr =%g\n", relerr);
00147             Vnm_print(2, "          rho   =%g\n", rho);
00148         }
00149
00150         if( relerr < *tol || *iters == *itmax)
00151             break;
00152
00153         oldrho = rho;
00154     }
00155 }
00156
00157 // Return some stuff ***
00158 *eigmax = rho;
00159 fac = VPOW(2.0, *ilev - 1);
00160 *eigmax_model = fac * (6.0 - 2.0 * VCOS((nx - 2) * pi / (nx - 1))
00161                      - 2.0 * VCOS((ny - 2) * pi / (ny - 1)));
00162 }
00163
00164
00165 VPUBLIC void Vipower(int *nx,int *ny,int *nz,
00166                    double *u, int *iz,
00167                    double *w0, double *w1, double *w2, double *w3, double *w4,
00168                    double *eigmin, double *eigmin_model, double *tol,
00169                    int *itmax, int *iters,
00170                    int *nlev, int *ilev, int *nlev_real, int *mgsolv,

```

```

00171     int *iok, int *iinfo, double *epsiln, double *errtol, double *omega,
00172     int *nul, int *nu2, int *mgsmoo,
00173     int *ipc, double *rpc,
00174     double *pc, double *ac, double *cc, double *tru) {
00175
00176     int level, lev;
00177     double denom, fac, rho, oldrho;
00178     double error, relerr, errtol_s;
00179     int itmax_s, iters_s, ierror_s, iok_s, iinfo_s, istop_s;
00180     int nul_s, nu2_s, mgsmoo_s;
00181
00182     double pi = 4.0 * atan( 1.0 );
00183
00184     // Utility variables
00185     double alpha;
00186
00187     MAT2(iz, 50, 1);
00188
00189     WARN_UNTESTED;
00190
00191     // Recover level information
00192     level = 1;
00193     lev = (*ilev - 1) + level;
00194
00195     // Seed vector: random to contain all components
00196     Vaxrand(nx, ny, nz, w1);
00197     Vazeros(nx, ny, nz, w2);
00198     Vazeros(nx, ny, nz, w3);
00199     Vazeros(nx, ny, nz, w4);
00200     Vazeros(nx, ny, nz, RAT(w0, VAT2(iz, 1, lev)));
00201     Vazeros(nx, ny, nz, RAT( u, VAT2(iz, 1, lev)));
00202
00203     // Compute raleigh quotient with the seed vector ***
00204     denom = Vxnorm2(nx, ny, nz, w1);
00205     fac = 1.0 / denom;
00206     Vxscal(nx, ny, nz, &fac, w1);
00207     Vmatvec(nx, ny, nz,
00208             RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00209             RAT( ac, VAT2(iz, 7, lev)), RAT( cc, VAT2(iz, 1, lev)), w1, w2);
00210     oldrho = Vxdot(nx, ny, nz, w1, w2);
00211
00212     // I/O
00213     if (oldrho == 0.0) {
00214         if (*iinfo > 3) {
00215             Vnm_print(2, "Vipower: iters=%d\n", *iters);
00216             Vnm_print(2, "estimate=%f\n", oldrho);
00217         }
00218         rho = oldrho;
00219     } else {
00220         //main iteration
00221         *iters = 0;
00222         while (1) {
00223             (*iters)++;
00224
00225             // Apply the matrix A^{-1} (using MG solver)
00226             itmax_s = 100;
00227             iters_s = 0;
00228             ierror_s = 0;
00229             iok_s = 0;
00230             iinfo_s = 0;
00231             istop_s = 0;
00232             mgsmoo_s = 1;
00233             nul_s = 1;
00234             nu2_s = 1;
00235             errtol_s = *epsiln;
00236
00237             Vxcopy(nx, ny, nz, w1, RAT(w0, VAT2(iz, 1, lev)));
00238             Vmvecs(nx, ny, nz, u, iz,
00239                   w1, w2, w3, w4,
00240                   &istop_s, &itmax_s, &iters_s, &ierror_s,
00241                   nlev, ilev, nlev_real, mgsolv,
00242                   &iok_s, &iinfo_s, epsiln,
00243                   &errtol_s, omega, &nul_s, &nu2_s, &mgsmoo_s,
00244                   ipc, rpc, pc, ac, cc, w0, tru);
00245             Vxcopy(nx, ny, nz, RAT(u, VAT2(iz, 1, lev)), w1);
00246
00247             // Normalize the new vector
00248             denom = Vxnorm2(nx, ny, nz, w1);
00249             fac = 1.0 / denom;
00250             Vxscal(nx, ny, nz, &fac, w1);
00251
00252

```

```

00253
00254 // Compute the new raleigh quotient
00255 Vmatvec(nx, ny, nz,
00256         RAT(ipc, VAT2(iz, 5, lev)), RAT(rpc, VAT2(iz, 6, lev)),
00257         RAT(ac, VAT2(iz, 7, lev)), RAT(cc, VAT2(iz, 1, lev)), w1, w2);
00258 rho = Vxdot(nx, ny, nz, w1, w2);
00259
00260 // Stopping test
00261 // w2=A*x, w1=x, stop = 2-norm(A*x-lamda*x) ***
00262 Vxcopy(nx, ny, nz, w1, w3);
00263 Vxcopy(nx, ny, nz, w2, w4);
00264 Vxscal(nx, ny, nz, &rho, w3);
00265 alpha = -1.0;
00266 Vxaxpy(nx, ny, nz, &alpha, w3, w4);
00267 error = Vxnorm2(nx, ny, nz, w4);
00268 relerr = VABS(rho - oldrho) / VABS(rho);
00269
00270 // I/O
00271 if (*iinfo > 3) {
00272
00273     Vnm_print(2, "POWER:  iters  =%d\n", *iters);
00274     Vnm_print(2, "          error  =%g\n", error);
00275     Vnm_print(2, "          relerr =%g\n", relerr);
00276     Vnm_print(2, "          rho   =%g\n", rho);
00277 }
00278
00279 if (relerr < *tol || *iters == *itmax)
00280     break;
00281
00282 oldrho = rho;
00283 }
00284 }
00285
00286 // Return some stuff
00287 *eigmin = rho;
00288 fac = VPOW(2.0, *ilev - 1);
00289 *eigmin_model = fac * (6.0 - 2.0 * VCOS(pi / (*nx - 1))
00290                      - 2.0 * VCOS(pi / (*ny - 1))
00291                      - 2.0 * VCOS(pi / (*nz - 1)));
00292 }
00293
00294 VEXTERNC void Vmpower(int *nx, int *ny, int *nz,
00295                      double *u, int *iz,
00296                      double *w0, double *w1, double *w2, double *w3, double *w4,
00297                      double *eigmax, double *tol,
00298                      int *itmax, int *iters, int *nlev, int *ilev, int *nlev_real,
00299                      int *mgsolv, int *iok, int *iinfo,
00300                      double *epsiln, double *errtol, double *omega,
00301                      int *nul, int *nu2, int *mgsmoo, int *ipc, double *rpc,
00302                      double *pc, double *ac, double *cc, double *fc, double *tru) {
00303
00304 // Local variables
00305 int lev, level;
00306 double denom, fac, rho, oldrho, error;
00307 double relerr;
00308 int itmax_s, iters_s, ierror_s, iok_s, iinfo_s, istop_s;
00309 double alpha;
00310
00311 MAT2(iz, 50, 1);
00312
00313 // Recover level information
00314 level = 1;
00315 lev = (*ilev - 1) + level;
00316
00317 // Seed vector: random to contain all components
00318 Vaxrand(nx, ny, nz, w1);
00319 Vazeros(nx, ny, nz, w2);
00320 Vazeros(nx, ny, nz, w3);
00321 Vazeros(nx, ny, nz, w4);
00322 Vazeros(nx, ny, nz, RAT(u, VAT2(iz, 1, lev)));
00323
00324 // NOTE: we destroy "fc" on this level due to lack of vectors... ***
00325 Vazeros(nx, ny, nz, RAT(fc, VAT2(iz, 1, lev)));
00326
00327 // Normalize the seed vector
00328 denom = Vxnorm2(nx, ny, nz, w1);
00329 fac = 1.0 / denom;
00330 Vxscal(nx, ny, nz, &fac, w1);
00331
00332 // Compute raleigh quotient with the seed vector
00333 Vxcopy(nx, ny, nz, w1, RAT(u, VAT2(iz, 1, lev)));

```

```

00334     itmax_s = 1;
00335     iters_s = 0;
00336     ierror_s = 0;
00337     iok_s = 0;
00338     iinfo_s = 0;
00339     istop_s = 1;
00340     Vmvecs(nx, ny, nz,
00341            u, iz, w0, w2, w3, w4,
00342            &istop_s, &itmax_s, &iters_s, &ierror_s,
00343            nlev, ilev, nlev_real, mgsolv,
00344            &iok_s, &iinfo_s,
00345            epsiln, errtol, omega, nul, nu2, mgsmoo,
00346            ipc, rpc,
00347            pc, ac, cc, fc, tru);
00348     oldrho = Vxdot(nx, ny, nz, w1, RAT(u, VAT2(iz, 1, lev)));
00349
00350     // I/O
00351     if (oldrho == 0.0) {
00352         if (*iinfo > 3) {
00353             Vnm_print(2, "Vmp0ower: iter=%d, estimate=%f", *iters, oldrho);
00354         }
00355         rho = oldrho;
00356     }
00357     else {
00358         // Main iteration
00359         *iters = 0;
00360         while (1) {
00361             (*iters)++;
00362
00363             // Apply the matrix M
00364             Vxcopy(nx, ny, nz, w1, RAT(u, VAT2(iz, 1, lev)));
00365             itmax_s = 1;
00366             iters_s = 0;
00367             ierror_s = 0;
00368             iok_s = 0;
00369             iinfo_s = 0;
00370             istop_s = 1;
00371             Vmvecs(nx, ny, nz,
00372                    u, iz, w1, w2, w3, w4,
00373                    &istop_s, &itmax_s, &iters_s, &ierror_s,
00374                    nlev, ilev, nlev_real, mgsolv,
00375                    &iok_s, &iinfo_s,
00376                    epsiln, errtol, omega, nul, nu2, mgsmoo,
00377                    ipc, rpc,
00378                    pc, ac, cc, fc, tru);
00379             Vxcopy(nx, ny, nz, RAT(u, VAT2(iz, 1, lev)), w1);
00380
00381             // Normalize the new vector
00382             denom = Vxnrm2(nx, ny, nz, w1);
00383             fac = 1.0 / denom;
00384             Vxscal(nx, ny, nz, &fac, w1);
00385
00386             // Compute the new raleigh quotient
00387             Vxcopy(nx, ny, nz, w1, RAT(u, VAT2(iz, 1, lev)));
00388             itmax_s = 1;
00389             iters_s = 0;
00390             ierror_s = 0;
00391             iok_s = 0;
00392             iinfo_s = 0;
00393             istop_s = 1;
00394             Vmvecs(nx, ny, nz,
00395                    u, iz, w0, w2, w3, w4,
00396                    &istop_s, &itmax_s, &iters_s, &ierror_s,
00397                    nlev, ilev, nlev_real, mgsolv,
00398                    &iok_s, &iinfo_s,
00399                    epsiln, errtol, omega, nul, nu2, mgsmoo,
00400                    ipc, rpc,
00401                    pc, ac, cc, fc, tru);
00402             Vxcopy(nx, ny, nz, RAT(u, VAT2(iz, 1, lev)), w2);
00403             rho = Vxdot(nx, ny, nz, w1, w2);
00404
00405             // Stopping test
00406             // w2=A*x, w1=x, stop = 2-norm(A*x-lamda*x)
00407             alpha = -1.0;
00408             Vxcopy(nx, ny, nz, w1, w3);
00409             Vxcopy(nx, ny, nz, w2, w4);
00410             Vxscal(nx, ny, nz, &rho, w3);
00411             Vxaxpy(nx, ny, nz, &alpha, w3, w4);
00412             error = Vxnrm2(nx, ny, nz, w4);
00413             relerr = VABS( rho - oldrho ) / VABS( rho );
00414

```

```

00415
00416         // I/O
00417         if (*iinfo > 3) {
00418             Vnm_print(2, "Vmpower: iter=%d; error=%f; relerr=%f; estimate=%f",
00419                 *iters, error, relerr, rho);
00420         }
00421
00422         if ((relerr < *tol) || (*iters == *itmax)) {
00423             break;
00424         }
00425
00426         oldrho = rho;
00427     }
00428 }
00429
00430 *eigmax = rho;
00431 }

```

9.147 powerd.h

```

00001
00049 #ifndef _POWERD_H_
00050 #define _POWERD_H_
00051
00052 #include "apbscfg.h"
00053
00054 #include "malloc/malloc.h"
00055
00056 #include "generic/vhal.h"
00057 #include "generic/vmatrix.h"
00058 #include "pmgc/mikpckd.h"
00059 #include "pmgc/mgcsd.h"
00060
00078 VEXTERNC void Vpower(
00079     int *nx,
00080     int *ny,
00081     int *nz,
00082     int *iz,
00083     int *ilev,
00084     int *ipc,
00085     double *rpc,
00086     double *ac,
00087     double *cc,
00088     double *w1,
00089     double *w2,
00090     double *w3,
00091     double *w4,
00092     double *eigmax,
00093     double *eigmax_model,
00094     double *tol,
00095     int *itmax,
00096     int *iters,
00097     int *iinfo
00098 );
00099
00100
00101
00119 VEXTERNC void Vipower(
00120     int *nx,
00121     int *ny,
00122     int *nz,
00123     double *u,
00124     int *iz,
00125     double *w0,
00126     double *w1,
00127     double *w2,
00128     double *w3,
00129     double *w4,
00130     double *eigmin,
00131     double *eigmin_model,
00132     double *tol,
00133     int *itmax,
00134     int *iters,
00135     int *nlev,
00136     int *ilev,
00137     int *nlev_real,
00138     int *mgsolv,
00139     int *iok,

```



```

00140         int *iinfo,
00141         double *epsiln,
00142         double *errtol,
00143         double *omega,
00144         int *nu1,
00145         int *nu2,
00146         int *mgsmoo,
00147         int *ipc,
00148         double *rpc,
00149         double *pc,
00150         double *ac,
00151         double *cc,
00152         double *tru
00153     );
00154
00155
00156
00157 VEXTERNC void Vmpower(
00158     int     *nx,
00159     int     *ny,
00160     int     *nz,
00161     double *u,
00162     int     *iz,
00163     double *w0,
00164     double *w1,
00165     double *w2,
00166     double *w3,
00167     double *w4,
00168     double *eigmax,
00169     double *tol,
00170     int     *itmax,
00171     int     *iters,
00172     int     *nlev,
00173     int     *ilev,
00174     int     *nlev_real,
00175     int     *mgsolv,
00176     int     *iok,
00177     int     *iinfo,
00178     double *epsiln,
00179     double *errtol,
00180     double *omega,
00181     int     *nu1,
00182     int     *nu2,
00183     int     *mgsmoo,
00184     int     *ipc,
00185     double *rpc,
00186     double *pc,
00187     double *ac,
00188     double *cc,
00189     double *fc,
00190     double *tru
00191 );
00192
00193 #endif /* _POWERD_H_ */

```

9.148 smoothd.c

```

00001
00056 #include "smoothd.h"
00057
00058 VEXTERNC void Vsmooth(int *nx, int *ny, int *nz,
00059     int *ipc, double *rpc,
00060     double *ac, double *cc, double *fc,
00061     double *x, double *w1, double *w2, double *r,
00062     int *itmax, int *iters,
00063     double *errtol, double *omega,
00064     int *iresid, int *iadjoint, int *meth) {
00065
00066     // Do in one step
00067     if (*meth == 0) {
00068         VABORT_MSG0( "wjac not yet translated" );
00069         //wjac(nx,ny,nz,ipc,rpc,ac,cc,fc,x,w1,w2,r,itmax,iters,errtol,omega,iresid,iadjoint);
00070     } else if (*meth == 1) {
00071         Vgsrb(nx, ny, nz,
00072             ipc, rpc,
00073             ac, cc, fc,
00074             x, w1, w2, r,
00075             itmax, iters,

```

```

00076         errtol, omega,
00077         iresid, iadjoint);
00078     } else if (*meth == 2) {
00079         VABORT_MSG0( "sor not yet translated" );
00080         //sor(nx,ny,nz,ipc,rpc,ac,cc,fc,x,w1,w2,r,itmax,itors,errtol,omega,iresid,iadjoint);
00081     } else if (*meth == 3) {
00082         VABORT_MSG0( "rich not yet translated" );
00083         //rich(nx,ny,nz,ipc,rpc,ac,cc,fc,x,w1,w2,r,itmax,itors,errtol,omega,iresid,iadjoint);
00084     } else if (*meth == 4) {
00085         Vcghs(nx, ny, nz,
00086             ipc, rpc,
00087             ac, cc, fc,
00088             x, w1, w2, r,
00089             itmax, iters,
00090             errtol, omega,
00091             iresid, iadjoint);
00092     } else {
00093         VABORT_MSG1("Bad smoothing routine specified = %d", *meth);
00094     }
00095 }
00096
00097
00098 VEXTERNC void Vnsmooth(int *nx, int *ny, int *nz,
00099     int *ipc, double *rpc,
00100     double *ac, double *cc, double *fc,
00101     double *x, double *w1, double *w2, double *r,
00102     int *itmax, int *itors,
00103     double *errtol, double *omega,
00104     int *iresid, int *iadjoint, int *meth) {
00105
00106     WARN_UNTESTED;
00107
00108     // Do in one step
00109     if (*meth == 0) {
00110         VABORT_MSG0( "nwjac not yet translated" );
00111         //nwjac(nx,ny,nz,ipc,rpc,ac,cc,fc,x,w1,w2,r,itmax,itors,errtol,omega,iresid,iadjoint)
00112     } else if (*meth == 1) {
00113         VABORT_MSG0( "ngsrb not yet translated" );
00114         //ngsrb(nx,ny,nz,ipc,rpc,ac,cc,fc,x,w1,w2,r,itmax,itors,errtol,omega,iresid,iadjoint)
00115     } else if (*meth == 2) {
00116         VABORT_MSG0( "nsor not yet translated" );
00117         //nsor(nx,ny,nz,ipc,rpc,ac,cc,fc,x,w1,w2,r,itmax,itors,errtol,omega,iresid,iadjoint)
00118     } else if (*meth == 3) {
00119         VABORT_MSG0( "nrich not yet translated" );
00120         //nrich(nx,ny,nz,ipc,rpc,ac,cc,fc,x,w1,w2,r,itmax,itors,errtol,omega,iresid,iadjoint)
00121     } else {
00122         VABORT_MSG1("Bad smoothing routine specified: %d", *meth );
00123     }
00124 }

```

9.149 smoothd.h

```

00001
00049 #ifndef _SMOOTHD_H_
00050 #define _SMOOTHD_H_
00051
00052 #include "apbscfg.h"
00053
00054 #include "malloc/malloc.h"
00055
00056 #include "generic/vhal.h"
00057 #include "generic/vmatrix.h"
00058 #include "pmgc/gsd.h"
00059 #include "pmgc/cgd.h"
00060
00067 VEXTERNC void Vsmooth(
00068     int *nx,
00069     int *ny,
00070     int *nz,
00071     int *ipc,
00072     double *rpc,
00073     double *ac,
00074     double *cc,
00075     double *fc,
00076     double *x,
00077     double *w1,
00078     double *w2,
00079     double *r,

```

```

00080         int      *itmax,
00081         int      *iters,
00082         double   *errtol,
00083         double   *omega,
00084         int      *iresid,
00085         int      *iadjoint,
00086         int      *meth
00087     );
00088
00095 VEXTERNC void Vnsmooth(
00096     int      *nx,
00097     int      *ny,
00098     int      *nz,
00099     int      *ipc,
00100     double   *rpc,
00101     double   *ac,
00102     double   *cc,
00103     double   *fc,
00104     double   *x,
00105     double   *w1,
00106     double   *w2,
00107     double   *r,
00108     int      *itmax,
00109     int      *iters,
00110     double   *errtol,
00111     double   *omega,
00112     int      *iresid,
00113     int      *iadjoint,
00114     int      *meth
00115 );
00116
00117
00118 #endif /* __SMOOTHD_H__ */

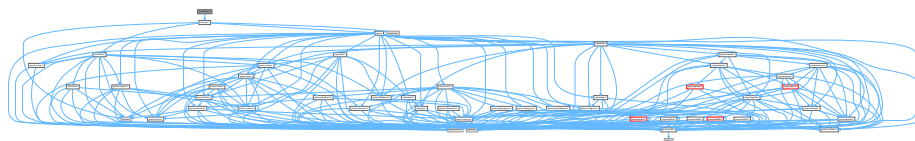
```

9.150 src/routines.c File Reference

Supporting routines for APBS front end.

```
#include "routines.h"
```

Include dependency graph for routines.c:



Functions

- VPUBLIC void [startVio](#) ()
Wrapper to start MALOC Vio layer.
- VPUBLIC [Vparam](#) * [loadParameter](#) ([NOsh](#) *nosh)
Loads and returns parameter object.
- VPUBLIC int [loadMolecules](#) ([NOsh](#) *nosh, [Vparam](#) *param, [Valist](#) *alist[[NOSH_MAXMOL](#)])
Load the molecules given in NOsh into atom lists.
- VPUBLIC void [killMolecules](#) ([NOsh](#) *nosh, [Valist](#) *alist[[NOSH_MAXMOL](#)])
Destroy the loaded molecules.
- VPUBLIC int [loadDielMaps](#) ([NOsh](#) *nosh, [Vgrid](#) *dielXMap[[NOSH_MAXMOL](#)], [Vgrid](#) *dielYMap[[NOSH_MAXMOL](#)], [Vgrid](#) *dielZMap[[NOSH_MAXMOL](#)])
Load the dielectric maps given in NOsh into grid objects.
- VPUBLIC void [killDielMaps](#) ([NOsh](#) *nosh, [Vgrid](#) *dielXMap[[NOSH_MAXMOL](#)], [Vgrid](#) *dielYMap[[NOSH_MAXMOL](#)], [Vgrid](#) *dielZMap[[NOSH_MAXMOL](#)])
Destroy the loaded dielectric.

- VPUBLIC int [loadKappaMaps](#) (NOSH *nosh, Vgrid *map[NOSH_MAXMOL])
Load the kappa maps given in NOSH into grid objects.
- VPUBLIC void [killKappaMaps](#) (NOSH *nosh, Vgrid *map[NOSH_MAXMOL])
Destroy the loaded kappa maps.
- VPUBLIC int [loadPotMaps](#) (NOSH *nosh, Vgrid *map[NOSH_MAXMOL])
Load the potential maps given in NOSH into grid objects.
- VPUBLIC void [killPotMaps](#) (NOSH *nosh, Vgrid *map[NOSH_MAXMOL])
Destroy the loaded potential maps.
- VPUBLIC int [loadChargeMaps](#) (NOSH *nosh, Vgrid *map[NOSH_MAXMOL])
Load the charge maps given in NOSH into grid objects.
- VPUBLIC void [killChargeMaps](#) (NOSH *nosh, Vgrid *map[NOSH_MAXMOL])
Destroy the loaded charge maps.
- VPUBLIC void [printPBEPARM](#) (PBEParm *pbeparm)
Print out generic PBE params loaded from input.
- VPUBLIC void [printMGPARM](#) (MGparm *mgparm, double realCenter[3])
Print out MG-specific params loaded from input.
- VPUBLIC int [initMG](#) (int icalc, NOSH *nosh, MGparm *mgparm, PBEParm *pbeparm, double realCenter[3], Vpbe *pbe[NOSH_MAXCALC], Valist *alist[NOSH_MAXMOL], Vgrid *dielXMap[NOSH_MAXMOL], Vgrid *dielYMap[NOSH_MAXMOL], Vgrid *dielZMap[NOSH_MAXMOL], Vgrid *kappaMap[NOSH_MAXMOL], Vgrid *chargeMap[NOSH_MAXMOL], Vpmgp *pmgp[NOSH_MAXCALC], Vpmg *pmg[NOSH_MAXCALC], Vgrid *potMap[NOSH_MAXMOL])
Initialize an MG calculation.
- VPUBLIC void [killMG](#) (NOSH *nosh, Vpbe *pbe[NOSH_MAXCALC], Vpmgp *pmgp[NOSH_MAXCALC], Vpmg *pmg[NOSH_MAXCALC])
Kill structures initialized during an MG calculation.
- VPUBLIC int [solveMG](#) (NOSH *nosh, Vpmg *pmg, MGparm_CalcType type)
Solve the PBE with MG.
- VPUBLIC int [setPartMG](#) (NOSH *nosh, MGparm *mgparm, Vpmg *pmg)
Set MG partitions for calculating observables and performing I/O.
- VPUBLIC int [energyMG](#) (NOSH *nosh, int icalc, Vpmg *pmg, int *nenergy, double *totEnergy, double *qfEnergy, double *qmEnergy, double *dielEnergy)
Calculate electrostatic energies from MG solution.
- VPUBLIC int [forceMG](#) (Vmem *mem, NOSH *nosh, PBEParm *pbeparm, MGparm *mgparm, Vpmg *pmg, int *nforce, AtomForce **atomForce, Valist *alist[NOSH_MAXMOL])
Calculate forces from MG solution.
- VPUBLIC void [killEnergy](#) ()
Kill arrays allocated for energies.
- VPUBLIC void [killForce](#) (Vmem *mem, NOSH *nosh, int nforce[NOSH_MAXCALC], AtomForce *atomForce[NOSH_MAXCALC])
Free memory from MG force calculation.
- VPUBLIC int [writematMG](#) (int rank, NOSH *nosh, PBEParm *pbeparm, Vpmg *pmg)
Write out operator matrix from MG calculation to file.
- VPUBLIC void [storeAtomEnergy](#) (Vpmg *pmg, int icalc, double **atomEnergy, int *nenergy)
Store energy in arrays for future use.
- VPUBLIC int [writedataFlat](#) (NOSH *nosh, Vcom *com, const char *fname, double totEnergy[NOSH_MAXCALC], double qfEnergy[NOSH_MAXCALC], double qmEnergy[NOSH_MAXCALC], double dielEnergy[NOSH_MAXCALC], int nenergy[NOSH_MAXCALC], double *atomEnergy[NOSH_MAXCALC], int nforce[NOSH_MAXCALC], AtomForce *atomForce[NOSH_MAXCALC])

Write out information to a flat file.

- VPUBLIC int [writedataXML](#) (NOSH *nosh, Vcom *com, const char *fname, double totEnergy[NOSH_MAXCALC], double qfEnergy[NOSH_MAXCALC], double qmEnergy[NOSH_MAXCALC], double dielEnergy[NOSH_MAXCALC], int nenergy[NOSH_MAXCALC], double *atomEnergy[NOSH_MAXCALC], int nforce[NOSH_MAXCALC], AtomForce *atomForce[NOSH_MAXCALC])

Write out information to an XML file.

- VPUBLIC int [writedataMG](#) (int rank, NOSH *nosh, PBEparm *pbeparm, Vpmg *pmg)

Write out observables from MG calculation to file.

- VPUBLIC double [returnEnergy](#) (Vcom *com, NOSH *nosh, double totEnergy[NOSH_MAXCALC], int iprint)

Access net local energy.

- VPUBLIC int [printEnergy](#) (Vcom *com, NOSH *nosh, double totEnergy[NOSH_MAXCALC], int iprint)

Combine and pretty-print energy data (deprecated...see printElecEnergy)

- VPUBLIC int [printElecEnergy](#) (Vcom *com, NOSH *nosh, double totEnergy[NOSH_MAXCALC], int iprint)

Combine and pretty-print energy data.

- VPUBLIC int [printApolEnergy](#) (NOSH *nosh, int iprint)

Combine and pretty-print energy data.

- VPUBLIC int [printForce](#) (Vcom *com, NOSH *nosh, int nforce[NOSH_MAXCALC], AtomForce *atomForce[NOSH_MAXCALC], int iprint)

Combine and pretty-print force data (deprecated...see printElecForce)

- VPUBLIC int [printElecForce](#) (Vcom *com, NOSH *nosh, int nforce[NOSH_MAXCALC], AtomForce *atomForce[NOSH_MAXCALC], int iprint)

Combine and pretty-print force data.

- VPUBLIC int [printApolForce](#) (Vcom *com, NOSH *nosh, int nforce[NOSH_MAXCALC], AtomForce *atomForce[NOSH_MAXCALC], int iprint)

Combine and pretty-print force data.

- VPUBLIC void [killFE](#) (NOSH *nosh, Vpbe *pbe[NOSH_MAXCALC], Vfetk *fetk[NOSH_MAXCALC], Gem *gm[NOSH_MAXMOL])

Kill structures initialized during an FE calculation.

- VPUBLIC Vrc_Codes [initFE](#) (int icalc, NOSH *nosh, FEMparm *feparm, PBEparm *pbeparm, Vpbe *pbe[NOSH_MAXCALC], Valist *alist[NOSH_MAXMOL], Vfetk *fetk[NOSH_MAXCALC])

Initialize FE solver objects.

- VPUBLIC void [printFEPARM](#) (int icalc, NOSH *nosh, FEMparm *feparm, Vfetk *fetk[NOSH_MAXCALC])

Print out FE-specific params loaded from input.

- VPUBLIC int [partFE](#) (int icalc, NOSH *nosh, FEMparm *feparm, Vfetk *fetk[NOSH_MAXCALC])

Partition mesh (if applicable)

- VPUBLIC int [preRefineFE](#) (int icalc, FEMparm *feparm, Vfetk *fetk[NOSH_MAXCALC])

Pre-refine mesh before solve.

- VPUBLIC int [solveFE](#) (int icalc, PBEparm *pbeparm, FEMparm *feparm, Vfetk *fetk[NOSH_MAXCALC])

Solve-estimate-refine.

- VPUBLIC int [energyFE](#) (NOSH *nosh, int icalc, Vfetk *fetk[NOSH_MAXCALC], int *nenergy, double *totEnergy, double *qfEnergy, double *qmEnergy, double *dielEnergy)

Calculate electrostatic energies from FE solution.

- VPUBLIC int [postRefineFE](#) (int icalc, FEMparm *feparm, Vfetk *fetk[NOSH_MAXCALC])

Estimate error, mark mesh, and refine mesh after solve.

- VPUBLIC int [writedataFE](#) (int rank, NOSH *nosh, PBEparm *pbeparm, Vfetk *fetk)

Write FEM data to files.

- VPUBLIC int [initAPOL](#) (NOSH *nosh, Vmem *mem, Vparam *param, APOLparm *apolparm, int *nforce, AtomForce **atomForce, Valist *alist)

Upperlevel routine to the non-polar energy and force routines.

- VPUBLIC int **energyAPOL** (**APOLparm** *apolparm, double sasa, double sav, double atomsasa[], double atomwcaEnergy[], int numatoms)

Calculate non-polar energies.

- VPUBLIC int **forceAPOL** (**Vacc** *acc, Vmem *mem, **APOLparm** *apolparm, int *nforce, **AtomForce** **atomForce, **Valist** *alist, **Vclist** *clist)

Calculate non-polar forces.

9.150.1 Detailed Description

Supporting routines for APBS front end.

Author

Nathan Baker

Version

\$Id\$

Attention

```
* APBS -- Adaptive Poisson-Boltzmann Solver
*
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*
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*
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```

```
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*
```

Definition in file [routines.c](#).

9.151 routines.c

[Go to the documentation of this file.](#)

```
00001
00054 #include "routines.h"
00055
00056 VEMBED(rcsid="$Id$")
00057
00058 VPUBLIC void startVio() { Vio_start(); }
00059
00060 VPUBLIC Vparam* loadParameter(NOsh *nosh) {
00061
00062     Vparam *param = VNULL;
00063
00064     if (nosh->gotparm) {
00065         param = Vparam_ctor();
00066         switch (nosh->parmfmt) {
00067             case NPF_FLAT:
00068                 Vnm_tprint( 1, "Reading parameter data from %s.\n",
00069                             nosh->parmpath);
00069                 if (Vparam_readFlatFile(param, "FILE", "ASC", VNULL,
00070                                         nosh->parmpath) != 1) {
00071                     Vnm_tprint(2, "Error reading parameter file (%s)!\n", nosh->parmpath);
00072                     return VNULL;
00073                 }
00074                 break;
00075             case NPF_XML:
00076                 Vnm_tprint( 1, "Reading parameter data from %s.\n",
00077                             nosh->parmpath);
00078                 if (Vparam_readXMLFile(param, "FILE", "ASC", VNULL,
00079                                         nosh->parmpath) != 1) {
00080                     Vnm_tprint(2, "Error reading parameter file (%s)!\n", nosh->parmpath);
00081                     return VNULL;
00082                 }
00083                 break;
00084             default:
00085                 Vnm_tprint(2, "Error! Undefined parameter file type (%d)!\n", nosh->parmfmt);
00086                 return VNULL;
00087         } /* switch parmfmt */
00088     }
00089
00090     return param;
00091 }
00092
00093
00094
00095 VPUBLIC int loadMolecules(NOsh *nosh, Vparam *param, Valist *alist[NOSH_MAXMOL]) {
00096
00097     int i;
00098     int use_params = 0;
00099     Vrc_Codes rc;
00100
00101     Vio *sock = VNULL;
00102
00103     Vnm_tprint( 1, "Got paths for %d molecules\n", nosh->nmol);
00104     if (nosh->nmol <= 0) {
00105         Vnm_tprint(2, "You didn't specify any molecules (correctly)!\n");
00106         Vnm_tprint(2, "Bailing out!\n");
00107         return 0;
00108     }
00109
00110     if (nosh->gotparm) {
00111         if (param == VNULL) {
00112             Vnm_tprint(2, "Error! You don't have a valid parameter object!\n");
00113             return 0;
00114         }
00115         use_params = 1;
00116     }
00117
00118     for (i=0; i<nosh->nmol; i++) {
00119         if (alist[i] == VNULL) {
00120             alist[i] = Valist_ctor();
```

```

00121     }else{
00122         alist[i] = VNULL;
00123         alist[i] = Valist_ctor();
00124     }
00125
00126     switch (nosh->molfmt[i]) {
00127         case NMF_PQR:
00128             /* Print out a warning to the user letting them know that we are overriding PQR
00129              values for charge, radius and epsilon */
00130             if (use_params) {
00131                 Vnm_print(2, "\nWARNING!! Radius/charge information from PQR file %s\n",
nosh->molpath[i]);
00132                 Vnm_print(2, "will be replaced with data from parameter file (%s)!\n",
nosh->parmpath);
00133             }
00134             Vnm_tprint( 1, "Reading PQR-format atom data from %s.\n",
nosh->molpath[i]);
00135             sock = Vio_ctor("FILE", "ASC", VNULL, nosh->molpath[i], "r");
00136             if (sock == VNULL) {
00137                 Vnm_print(2, "Problem opening virtual socket %s!\n",
nosh->molpath[i]);
00138                 return 0;
00139             }
00140             if (Vio_accept(sock, 0) < 0) {
00141                 Vnm_print(2, "Problem accepting virtual socket %s!\n",
nosh->molpath[i]);
00142                 return 0;
00143             }
00144             if (use_params) {
00145                 rc = Valist_readPQR(alist[i], param, sock);
00146             }else{
00147                 rc = Valist_readPQR(alist[i], VNULL, sock);
00148             }
00149             if(rc == 0) return 0;
00150
00151             Vio_acceptFree(sock);
00152             Vio_dtor(&sock);
00153             break;
00154         case NMF_PDB:
00155             /* Load parameters */
00156             if (!nosh->gotparm) {
00157                 Vnm_tprint(2, "Nosh: Error! Can't read PDB without specifying PARM file!\n");
00158                 return 0;
00159             }
00160             Vnm_tprint( 1, "Reading PDB-format atom data from %s.\n",
nosh->molpath[i]);
00161             sock = Vio_ctor("FILE", "ASC", VNULL, nosh->molpath[i], "r");
00162             if (sock == VNULL) {
00163                 Vnm_print(2, "Problem opening virtual socket %s!\n",
nosh->molpath[i]);
00164                 return 0;
00165             }
00166             if (Vio_accept(sock, 0) < 0) {
00167                 Vnm_print(2, "Problem accepting virtual socket %s!\n", nosh->molpath[i]);
00168                 return 0;
00169             }
00170             rc = Valist_readPDB(alist[i], param, sock);
00171             /* If we are looking for an atom/residue that does not exist
00172              * then abort and return 0 */
00173             if(rc == 0)
00174                 return 0;
00175
00176             Vio_acceptFree(sock);
00177             Vio_dtor(&sock);
00178             break;
00179         case NMF_XML:
00180             Vnm_tprint( 1, "Reading XML-format atom data from %s.\n",
nosh->molpath[i]);
00181             sock = Vio_ctor("FILE", "ASC", VNULL, nosh->molpath[i], "r");
00182             if (sock == VNULL) {
00183                 Vnm_print(2, "Problem opening virtual socket %s!\n",
nosh->molpath[i]);
00184                 return 0;
00185             }
00186             if (Vio_accept(sock, 0) < 0) {
00187                 Vnm_print(2, "Problem accepting virtual socket %s!\n",
nosh->molpath[i]);
00188                 return 0;
00189             }
00190             if (use_params) {
00191                 rc = Valist_readXML(alist[i], param, sock);

```



```
00200         }else{
00201             rc = Valist_readXML(alist[i], VNULL, sock);
00202         }
00203         if(rc == 0)
00204             return 0;
00205
00206         Vio_acceptFree(sock);
00207         Vio_dtor(&sock);
00208         break;
00209     default:
00210         Vnm_tprint(2, "Nosh: Error! Undefined molecule file type \
00211 (%d)!\n", nosh->molfmt[i]);
00212         return 0;
00213     } /* switch molfmt */
00214
00215     if (rc != 1) {
00216         Vnm_tprint( 2, "Error while reading molecule from %s\n",
00217             nosh->molpath[i]);
00218         return 0;
00219     }
00220
00221     Vnm_tprint( 1, " %d atoms\n", Valist_getNumberAtoms(alist[i]));
00222     Vnm_tprint( 1, "   Centered at (%4.3e, %4.3e, %4.3e)\n",
00223         alist[i]->center[0], alist[i]->center[1],
00224         alist[i]->center[2]);
00225     Vnm_tprint( 1, "   Net charge %3.2e e\n", alist[i]->charge);
00226
00227 }
00228
00229 return 1;
00230
00231 }
00232
00233 VPUBLIC void killMolecules(NOsh *nosh, Valist *alist[NOSH_MAXMOL]) {
00234
00235     int i;
00236
00237     #ifndef VAPBSQUIET
00238         Vnm_tprint( 1, "Destroying %d molecules\n", nosh->nmol);
00239     #endif
00240
00241     for (i=0; i<nosh->nmol; i++)
00242         Valist_dtor(&(alist[i]));
00243
00244 }
00245
00250 VPUBLIC int loadDielMaps(NOsh *nosh, Vgrid *dielXMap[NOSH_MAXMOL], Vgrid *dielYMap[NOSH_MAXMOL], Vgrid
    *dielZMap[NOSH_MAXMOL]){
00251
00252     int i,ii,nx,ny,nz;
00253     double sum,hx,hy,hzed,xmin,ymin,zmin;
00254
00255     // Check to be sure we have dielectric map paths; if not, return.
00256     if (nosh->ndiel > 0)
00257         Vnm_tprint( 1, "Got paths for %d dielectric map sets\n",nosh->ndiel);
00258     else
00259         return 1;
00260
00261     // For each dielectric map path, read the data and calculate needed values.
00262     for (i=0; i<nosh->ndiel; i++) {
00263         Vnm_tprint( 1, "Reading x-shifted dielectric map data from %s:\n", nosh->dielXpath[i]);
00264         dielXMap[i] = Vgrid_ctor(0, 0, 0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, VNULL);
00265
00266         // Determine the format and read data if the format is valid.
00267         switch (nosh->dielfmt[i]) {
00268             // OpenDX (Data Explorer) format
00269             case VDF_DX:
00270                 if (Vgrid_readDX(dielXMap[i], "FILE", "ASC", VNULL,
00271                     nosh->dielXpath[i]) != 1) {
00272                     Vnm_tprint( 2, "Fatal error while reading from %s\n",
00273                         nosh->dielXpath[i]);
00274                     return 0;
00275                 }
00276
00277                 // Set grid sizes
00278                 nx = dielXMap[i]->nx;
00279                 ny = dielXMap[i]->ny;
00280                 nz = dielXMap[i]->nz;
00281
00282                 // Set spacings
00283                 hx = dielXMap[i]->hx;
```

```

00284         hy = dielXMap[i]->hy;
00285         hzed = dielXMap[i]->hzed;
00286
00287         // Set minimum lower corner
00288         xmin = dielXMap[i]->xmin;
00289         ymin = dielXMap[i]->ymin;
00290         zmin = dielXMap[i]->zmin;
00291         Vnm_tprint(1, " %d x %d x %d grid\n", nx, ny, nz);
00292         Vnm_tprint(1, " (%g, %g, %g) A spacings\n", hx, hy, hzed);
00293         Vnm_tprint(1, " (%g, %g, %g) A lower corner\n",
00294                   xmin, ymin, zmin);
00295         sum = 0;
00296         for (ii=0; ii<(nx*ny*nz); ii++)
00297             sum += (dielXMap[i]->data[ii]);
00298         sum = sum*hx*hy*hzed;
00299         Vnm_tprint(1, " Volume integral = %3.2e A^3\n", sum);
00300         break;
00301
00302         //DX binary file (.dxbin)
00303         case VDF_DXBIN:
00304             //TODO: add this method and maybe change the if stmt.
00305             if (Vgrid_readDXBIN(dielXMap[i], "FILE", "ASC", VNULL,
00306                               nosh->dielXpath[i]) != 1) {
00307                 Vnm_tprint( 2, "Fatal error while reading from %s\n",
00308                           nosh->dielXpath[i]);
00309                 return 0;
00310             }
00311
00312             // Set grid sizes
00313             nx = dielXMap[i]->nx;
00314             ny = dielXMap[i]->ny;
00315             nz = dielXMap[i]->nz;
00316
00317             // Set spacings
00318             hx = dielXMap[i]->hx;
00319             hy = dielXMap[i]->hy;
00320             hzed = dielXMap[i]->hzed;
00321
00322             // Set minimum lower corner
00323             xmin = dielXMap[i]->xmin;
00324             ymin = dielXMap[i]->ymin;
00325             zmin = dielXMap[i]->zmin;
00326             Vnm_tprint(1, " %d x %d x %d grid\n", nx, ny, nz);
00327             Vnm_tprint(1, " (%g, %g, %g) A spacings\n", hx, hy, hzed);
00328             Vnm_tprint(1, " (%g, %g, %g) A lower corner\n",
00329                       xmin, ymin, zmin);
00330             sum = 0;
00331             for (ii=0; ii<(nx*ny*nz); ii++)
00332                 sum += (dielXMap[i]->data[ii]);
00333             sum = sum*hx*hy*hzed;
00334             Vnm_tprint(1, " Volume integral = %3.2e A^3\n", sum);
00335             break;
00336
00337         // Binary file (GZip)
00338         case VDF_GZ:
00339             if (Vgrid_readGZ(dielXMap[i], nosh->dielXpath[i]) != 1) {
00340                 Vnm_tprint( 2, "Fatal error while reading from %s\n",
00341                           nosh->dielXpath[i]);
00342                 return 0;
00343             }
00344
00345             // Set grid sizes
00346             nx = dielXMap[i]->nx;
00347             ny = dielXMap[i]->ny;
00348             nz = dielXMap[i]->nz;
00349
00350             // Set spacings
00351             hx = dielXMap[i]->hx;
00352             hy = dielXMap[i]->hy;
00353             hzed = dielXMap[i]->hzed;
00354
00355             // Set minimum lower corner
00356             xmin = dielXMap[i]->xmin;
00357             ymin = dielXMap[i]->ymin;
00358             zmin = dielXMap[i]->zmin;
00359             Vnm_tprint(1, " %d x %d x %d grid\n", nx, ny, nz);
00360             Vnm_tprint(1, " (%g, %g, %g) A spacings\n", hx, hy, hzed);
00361             Vnm_tprint(1, " (%g, %g, %g) A lower corner\n",
00362                       xmin, ymin, zmin);
00363             sum = 0;
00364             for (ii=0; ii<(nx*ny*nz); ii++)

```

```

00365         sum += (dielXMap[i]->data[ii]);
00366         sum = sum*hx*hy*hzed;
00367         Vnm_tprint(1, " Volume integral = %3.2e A^3\n", sum);
00368         break;
00369         // UHBD format
00370         case VDF_UHBD:
00371             Vnm_tprint( 2, "UHBD input not supported yet!\n");
00372             return 0;
00373         // AVS UCD format
00374         case VDF_AVS:
00375             Vnm_tprint( 2, "AVS input not supported yet!\n");
00376             return 0;
00377         // FETk MC Simplex Format (MCSF)
00378         case VDF_MCSF:
00379             Vnm_tprint( 2, "MCSF input not supported yet!\n");
00380             return 0;
00381         default:
00382             Vnm_tprint( 2, "Invalid data format (%d)!\n",
00383                 nosh->dielfmt[i]);
00384             return 0;
00385     }
00386     Vnm_tprint( 1, "Reading y-shifted dielectric map data from \
00387 %s:\n", nosh->dielYpath[i]);
00388     dielYMap[i] = Vgrid_ctor(0, 0, 0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, VNULL);
00389
00390     // Determine the format and read data if the format is valid.
00391     switch (nosh->dielfmt[i]) {
00392         // OpenDX (Data Explorer) format
00393         case VDF_DX:
00394             if (Vgrid_readDX(dielYMap[i], "FILE", "ASC", VNULL,
00395                 nosh->dielYpath[i]) != 1) {
00396                 Vnm_tprint( 2, "Fatal error while reading from %s\n",
00397                     nosh->dielYpath[i]);
00398                 return 0;
00399             }
00400
00401             // Read grid
00402             nx = dielYMap[i]->nx;
00403             ny = dielYMap[i]->ny;
00404             nz = dielYMap[i]->nz;
00405
00406             // Read spacings
00407             hx = dielYMap[i]->hx;
00408             hy = dielYMap[i]->hy;
00409             hzed = dielYMap[i]->hzed;
00410
00411             // Read minimum lower corner
00412             xmin = dielYMap[i]->xmin;
00413             ymin = dielYMap[i]->ymin;
00414             zmin = dielYMap[i]->zmin;
00415             Vnm_tprint(1, " %d x %d x %d grid\n", nx, ny, nz);
00416             Vnm_tprint(1, " (%g, %g, %g) A spacings\n", hx, hy, hzed);
00417             Vnm_tprint(1, " (%g, %g, %g) A lower corner\n",
00418                 xmin, ymin, zmin);
00419             sum = 0;
00420             for (ii=0; ii<(nx*ny*nz); ii++)
00421                 sum += (dielYMap[i]->data[ii]);
00422             sum = sum*hx*hy*hzed;
00423             Vnm_tprint(1, " Volume integral = %3.2e A^3\n", sum);
00424             break;
00425         //DX Binary file (.dxbin)
00426         case VDF_DXBIN:
00427             //TODO: add this funct/method and maybe change the if stmt.
00428             if (Vgrid_readDXBIN(dielYMap[i], "FILE", "ASC", VNULL,
00429                 nosh->dielYpath[i]) != 1) {
00430                 Vnm_tprint( 2, "Fatal error while reading from %s\n",
00431                     nosh->dielYpath[i]);
00432                 return 0;
00433             }
00434
00435             // Read grid
00436             nx = dielYMap[i]->nx;
00437             ny = dielYMap[i]->ny;
00438             nz = dielYMap[i]->nz;
00439
00440             // Read spacings
00441             hx = dielYMap[i]->hx;
00442             hy = dielYMap[i]->hy;
00443             hzed = dielYMap[i]->hzed;
00444
00445             // Read minimum lower corner

```

```

00446     xmin = dielYMap[i]->xmin;
00447     ymin = dielYMap[i]->ymin;
00448     zmin = dielYMap[i]->zmin;
00449     Vnm_tprint(1, "    %d x %d x %d grid\n", nx, ny, nz);
00450     Vnm_tprint(1, "    (%g, %g, %g) A spacings\n", hx, hy, hzed);
00451     Vnm_tprint(1, "    (%g, %g, %g) A lower corner\n",
00452               xmin, ymin, zmin);
00453     sum = 0;
00454     for (ii=0; ii<(nx*ny*nz); ii++)
00455         sum += (dielYMap[i]->data[ii]);
00456     sum = sum*hx*hy*hzed;
00457     Vnm_tprint(1, "    Volume integral = %3.2e A^3\n", sum);
00458     break;
00459     // Binary file (GZip) format
00460     case VDF_GZ:
00461         if (Vgrid_readGZ(dielYMap[i], nosh->dielYpath[i]) != 1) {
00462             Vnm_tprint( 2, "Fatal error while reading from %s\n",
00463                       nosh->dielYpath[i]);
00464             return 0;
00465         }
00466
00467         // Read grid
00468         nx = dielYMap[i]->nx;
00469         ny = dielYMap[i]->ny;
00470         nz = dielYMap[i]->nz;
00471
00472         // Read spacings
00473         hx = dielYMap[i]->hx;
00474         hy = dielYMap[i]->hy;
00475         hzed = dielYMap[i]->hzed;
00476
00477         // Read minimum lower corner
00478         xmin = dielYMap[i]->xmin;
00479         ymin = dielYMap[i]->ymin;
00480         zmin = dielYMap[i]->zmin;
00481         Vnm_tprint(1, "    %d x %d x %d grid\n", nx, ny, nz);
00482         Vnm_tprint(1, "    (%g, %g, %g) A spacings\n", hx, hy, hzed);
00483         Vnm_tprint(1, "    (%g, %g, %g) A lower corner\n",
00484                   xmin, ymin, zmin);
00485         sum = 0;
00486         for (ii=0; ii<(nx*ny*nz); ii++)
00487             sum += (dielYMap[i]->data[ii]);
00488         sum = sum*hx*hy*hzed;
00489         Vnm_tprint(1, "    Volume integral = %3.2e A^3\n", sum);
00490         break;
00491     // UHBD format
00492     case VDF_UHBD:
00493         Vnm_tprint( 2, "UHBD input not supported yet!\n");
00494         return 0;
00495     // AVS UCD format
00496     case VDF_AVS:
00497         Vnm_tprint( 2, "AVS input not supported yet!\n");
00498         return 0;
00499     // FEtk MC Simplex Format (MCSF)
00500     case VDF_MCSF:
00501         Vnm_tprint( 2, "MCSF input not supported yet!\n");
00502         return 0;
00503     default:
00504         Vnm_tprint( 2, "Invalid data format (%d)!\n",
00505                   nosh->dielfmt[i]);
00506         return 0;
00507 }
00508
00509 Vnm_tprint( 1, "Reading z-shifted dielectric map data from \
00510 %s:\n", nosh->dielZpath[i]);
00511 dielZMap[i] = Vgrid_ctor(0, 0, 0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, VNULL);
00512
00513 // Determine the format and read data if the format is valid.
00514 switch (nosh->dielfmt[i]) {
00515     // OpenDX (Data Explorer) format
00516     case VDF_DX:
00517         if (Vgrid_readDX(dielZMap[i], "FILE", "ASC", VNULL,
00518                         nosh->dielZpath[i]) != 1) {
00519             Vnm_tprint( 2, "Fatal error while reading from %s\n",
00520                       nosh->dielZpath[i]);
00521             return 0;
00522         }
00523
00524         // Read grid
00525         nx = dielZMap[i]->nx;
00526         ny = dielZMap[i]->ny;

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00527         nz = dielZMap[i]->nz;
00528
00529         // Read spacings
00530         hx = dielZMap[i]->hx;
00531         hy = dielZMap[i]->hy;
00532         hzed = dielZMap[i]->hzed;
00533
00534         // Read minimum lower corner
00535         xmin = dielZMap[i]->xmin;
00536         ymin = dielZMap[i]->ymin;
00537         zmin = dielZMap[i]->zmin;
00538         Vnm_tprint(1, " %d x %d x %d grid\n",
00539                 nx, ny, nz);
00540         Vnm_tprint(1, " (%g, %g, %g) A spacings\n",
00541                 hx, hy, hzed);
00542         Vnm_tprint(1, " (%g, %g, %g) A lower corner\n",
00543                 xmin, ymin, zmin);
00544         sum = 0;
00545         for (ii=0; ii<(nx*ny*nz); ii++) sum += (dielZMap[i]->data[ii]);
00546         sum = sum*hx*hy*hzed;
00547         Vnm_tprint(1, " Volume integral = %3.2e A^3\n", sum);
00548         break;
00549         //OpenDX Binary format (.dxbn)
00550         case VDF_DXBIN:
00551             //TODO: add this funct/method and maybe change the if stmt.
00552             if (Vgrid_readDXBIN(dielZMap[i], "FILE", "ASC", VNULL,
00553                     nosh->dielZpath[i]) != 1) {
00554                 Vnm_tprint( 2, "Fatal error while reading from %s\n",
00555                         nosh->dielZpath[i]);
00556                 return 0;
00557             }
00558
00559         // Read grid
00560         nx = dielZMap[i]->nx;
00561         ny = dielZMap[i]->ny;
00562         nz = dielZMap[i]->nz;
00563
00564         // Read spacings
00565         hx = dielZMap[i]->hx;
00566         hy = dielZMap[i]->hy;
00567         hzed = dielZMap[i]->hzed;
00568
00569         // Read minimum lower corner
00570         xmin = dielZMap[i]->xmin;
00571         ymin = dielZMap[i]->ymin;
00572         zmin = dielZMap[i]->zmin;
00573         Vnm_tprint(1, " %d x %d x %d grid\n",
00574                 nx, ny, nz);
00575         Vnm_tprint(1, " (%g, %g, %g) A spacings\n",
00576                 hx, hy, hzed);
00577         Vnm_tprint(1, " (%g, %g, %g) A lower corner\n",
00578                 xmin, ymin, zmin);
00579         sum = 0;
00580         for (ii=0; ii<(nx*ny*nz); ii++) sum += (dielZMap[i]->data[ii]);
00581         sum = sum*hx*hy*hzed;
00582         Vnm_tprint(1, " Volume integral = %3.2e A^3\n", sum);
00583         break;
00584         // Binary file (GZip) format
00585         case VDF_GZ:
00586             if (Vgrid_readGZ(dielZMap[i], nosh->dielZpath[i]) != 1) {
00587                 Vnm_tprint( 2, "Fatal error while reading from %s\n",
00588                         nosh->dielZpath[i]);
00589                 return 0;
00590             }
00591
00592         // Read grid
00593         nx = dielZMap[i]->nx;
00594         ny = dielZMap[i]->ny;
00595         nz = dielZMap[i]->nz;
00596
00597         // Read spacings
00598         hx = dielZMap[i]->hx;
00599         hy = dielZMap[i]->hy;
00600         hzed = dielZMap[i]->hzed;
00601
00602         // Read minimum lower corner
00603         xmin = dielZMap[i]->xmin;
00604         ymin = dielZMap[i]->ymin;
00605         zmin = dielZMap[i]->zmin;
00606         Vnm_tprint(1, " %d x %d x %d grid\n",
00607                 nx, ny, nz);

```

```

00608         Vnm_tprint(1, " (%g, %g, %g) A spacings\n",
00609                     hx, hy, hzed);
00610         Vnm_tprint(1, " (%g, %g, %g) A lower corner\n",
00611                     xmin, ymin, zmin);
00612         sum = 0;
00613         for (ii=0; ii<(nx*ny*nz); ii++) sum += (dielZMap[ii]->data[ii]);
00614         sum = sum*hx*hy*hzed;
00615         Vnm_tprint(1, " Volume integral = %3.2e A^3\n", sum);
00616         break;
00617     // UHBD format
00618     case VDF_UHBD:
00619         Vnm_tprint( 2, "UHBD input not supported yet!\n");
00620         return 0;
00621     // AVS UCD format
00622     case VDF_AVS:
00623         Vnm_tprint( 2, "AVS input not supported yet!\n");
00624         return 0;
00625     // FETk MC Simplex Format (MCSF)
00626     case VDF_MCSF:
00627         Vnm_tprint( 2, "MCSF input not supported yet!\n");
00628         return 0;
00629     default:
00630         Vnm_tprint( 2, "Invalid data format (%d)!\n",
00631                     nosh->dielfmt[i]);
00632         return 0;
00633     }
00634 }
00635
00636 return 1;
00637 }
00638
00639 VPUBLIC void killDielMaps(NOSH *nosh,
00640                          Vgrid *dielXMap[NOSH_MAXMOL],
00641                          Vgrid *dielYMap[NOSH_MAXMOL],
00642                          Vgrid *dielZMap[NOSH_MAXMOL]) {
00643
00644     int i;
00645
00646     if (nosh->ndiel > 0) {
00647 #ifndef VAPBSQUIET
00648         Vnm_tprint( 1, "Destroying %d dielectric map sets\n",
00649                     nosh->ndiel);
00650 #endif
00651         for (i=0; i<nosh->ndiel; i++) {
00652             Vgrid_dtor(&(dielXMap[i]));
00653             Vgrid_dtor(&(dielYMap[i]));
00654             Vgrid_dtor(&(dielZMap[i]));
00655         }
00656     }
00657     else return;
00658 }
00659
00660 VPUBLIC int loadKappaMaps(NOSH *nosh,
00661                          Vgrid *map[NOSH_MAXMOL]) {
00662
00663     int i,
00664         ii,
00665         len;
00666     double sum;
00667
00668     if (nosh->nkappa > 0)
00669         Vnm_tprint( 1, "Got paths for %d kappa maps\n", nosh->nkappa);
00670     else return 1;
00671
00672     for (i=0; i<nosh->nkappa; i++) {
00673         Vnm_tprint( 1, "Reading kappa map data from %s:\n",
00674                     nosh->kappapath[i]);
00675         map[i] = Vgrid_ctor(0, 0, 0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, VNULL);
00676
00677         // Determine the format and read data if the format is valid.
00678         switch (nosh->kappafmt[i]) {
00679             // OpenDX (Data Explorer) format
00680             case VDF_DX:
00681                 if (Vgrid_readDX(map[i], "FILE", "ASC", VNULL,
00682                                 nosh->kappapath[i]) != 1) {
00683                     Vnm_tprint( 2, "Fatal error while reading from %s\n",
00684                                 nosh->kappapath[i]);
00685                     return 0;
00686                 }
00687             }
00688     }
00689 }

```

```

00692         Vnm_tprint(1, "  %d x %d x %d grid\n",
00693                     map[i]->nx, map[i]->ny, map[i]->nz);
00694         Vnm_tprint(1, "    (%g, %g, %g) A spacings\n",
00695                     map[i]->hx, map[i]->hy, map[i]->hz);
00696         Vnm_tprint(1, "    (%g, %g, %g) A lower corner\n",
00697                     map[i]->xmin, map[i]->ymin, map[i]->zmin);
00698         sum = 0;
00699         for (ii = 0, len = map[i]->nx * map[i]->ny * map[i]->nz;
00700             ii < len;
00701             ii++)
00702             ) {
00703             sum += (map[i]->data[ii]);
00704         }
00705         sum = sum*map[i]->hx*map[i]->hy*map[i]->hz;
00706         Vnm_tprint(1, " Volume integral = %3.2e A^3\n", sum);
00707         break;
00708         // OpenDX Binary (.dxbn) format
00709     case VDF_DXBIN:
00710         //TODO: write method and possible change if stmt.
00711         if (Vgrid_readDXBIN(map[i], "FILE", "ASC", VNULL,
00712                             nosh->kappapath[i]) != 1) {
00713             Vnm_tprint( 2, "Fatal error while reading from %s\n",
00714                         nosh->kappapath[i]);
00715             return 0;
00716         }
00717         Vnm_tprint(1, "  %d x %d x %d grid\n",
00718                     map[i]->nx, map[i]->ny, map[i]->nz);
00719         Vnm_tprint(1, "    (%g, %g, %g) A spacings\n",
00720                     map[i]->hx, map[i]->hy, map[i]->hz);
00721         Vnm_tprint(1, "    (%g, %g, %g) A lower corner\n",
00722                     map[i]->xmin, map[i]->ymin, map[i]->zmin);
00723         sum = 0;
00724         for (ii = 0, len = map[i]->nx * map[i]->ny * map[i]->nz;
00725             ii < len;
00726             ii++)
00727             ) {
00728             sum += (map[i]->data[ii]);
00729         }
00730         sum = sum*map[i]->hx*map[i]->hy*map[i]->hz;
00731         Vnm_tprint(1, " Volume integral = %3.2e A^3\n", sum);
00732         break;
00733         // UHBD format
00734     case VDF_UHBD:
00735         Vnm_tprint( 2, "UHBD input not supported yet!\n");
00736         return 0;
00737         // FETk MC Simplex Format (MCSF)
00738     case VDF_MCSF:
00739         Vnm_tprint( 2, "MCSF input not supported yet!\n");
00740         return 0;
00741         // AVS UCD format
00742     case VDF_AVS:
00743         Vnm_tprint( 2, "AVS input not supported yet!\n");
00744         return 0;
00745         // Binary file (GZip) format
00746     case VDF_GZ:
00747         if (Vgrid_readGZ(map[i], nosh->kappapath[i]) != 1) {
00748             Vnm_tprint( 2, "Fatal error while reading from %s\n",
00749                         nosh->kappapath[i]);
00750             return 0;
00751         }
00752         Vnm_tprint(1, "  %d x %d x %d grid\n",
00753                     map[i]->nx, map[i]->ny, map[i]->nz);
00754         Vnm_tprint(1, "    (%g, %g, %g) A spacings\n",
00755                     map[i]->hx, map[i]->hy, map[i]->hz);
00756         Vnm_tprint(1, "    (%g, %g, %g) A lower corner\n",
00757                     map[i]->xmin, map[i]->ymin, map[i]->zmin);
00758         sum = 0;
00759         for (ii=0, len=map[i]->nx*map[i]->ny*map[i]->nz; ii<len; ii++) {
00760             sum += (map[i]->data[ii]);
00761         }
00762         sum = sum*map[i]->hx*map[i]->hy*map[i]->hz;
00763         Vnm_tprint(1, " Volume integral = %3.2e A^3\n", sum);
00764         break;
00765     default:
00766         Vnm_tprint( 2, "Invalid data format (%d)!\n",
00767                     nosh->kappafmt[i]);
00768         return 0;
00769     }
00770 }
00771
00772 return 1;

```

```

00773
00774 }
00775
00776 VPUBLIC void killKappaMaps(NOsh *nosh, Vgrid *map[NOSH_MAXMOL]) {
00777     int i;
00778     if (nosh->nkappa > 0) {
00780         #ifndef VAPBSQUIET
00781             Vnm_tprint( 1, "Destroying %d kappa maps\n", nosh->nkappa);
00782         #endif
00783         for (i=0; i<nosh->nkappa; i++) Vgrid_dtor(&(map[i]));
00784     }
00785     else return;
00786 }
00787
00788 }
00789
00793 VPUBLIC int loadPotMaps(NOsh *nosh,
00794                         Vgrid *map[NOSH_MAXMOL]
00795                         ) {
00796     int i,
00797         ii,
00798         len;
00799     double sum;
00800
00801     if (nosh->npot > 0)
00802         Vnm_tprint( 1, "Got paths for %d potential maps\n", nosh->npot);
00803     else return 1;
00804
00805     for (i=0; i<nosh->npot; i++) {
00806         Vnm_tprint( 1, "Reading potential map data from %s:\n",
00807                     nosh->potpath[i]);
00808         map[i] = Vgrid_ctor(0, 0, 0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, VNULL);
00809         switch (nosh->potfmt[i]) {
00810             // OpenDX (Data Explorer) format
00811             case VDF_DX:
00812                 // Binary file (GZip) format
00813                 case VDF_GZ:
00814                     if (nosh->potfmt[i] == VDF_DX) {
00815                         if (Vgrid_readDX(map[i], "FILE", "ASC", VNULL,
00816                                         nosh->potpath[i]) != 1) {
00817                             Vnm_tprint( 2, "Fatal error while reading from %s\n",
00818                                         nosh->potpath[i]);
00819                             return 0;
00820                         }
00821                     } else {
00822                         if (Vgrid_readGZ(map[i], nosh->potpath[i]) != 1) {
00823                             Vnm_tprint( 2, "Fatal error while reading from %s\n",
00824                                         nosh->potpath[i]);
00825                             return 0;
00826                         }
00827                     }
00828                 Vnm_tprint(1, "  %d x %d x %d grid\n",
00829                             map[i]->nx, map[i]->ny, map[i]->nz);
00830                 Vnm_tprint(1, "  (%g, %g, %g) A spacings\n",
00831                             map[i]->hx, map[i]->hy, map[i]->hz);
00832                 Vnm_tprint(1, "  (%g, %g, %g) A lower corner\n",
00833                             map[i]->xmin, map[i]->ymin, map[i]->zmin);
00834                 sum = 0;
00835                 for (ii=0, len=map[i]->nx*map[i]->ny*map[i]->nz; ii<len; ii++) {
00836                     sum += (map[i]->data[ii]);
00837                 }
00838                 sum = sum*map[i]->hx*map[i]->hy*map[i]->hz;
00839                 Vnm_tprint(1, "  Volume integral = %3.2e A^3\n", sum);
00840                 break;
00841             // UHBD format
00842             case VDF_UHBD:
00843                 Vnm_tprint( 2, "UHBD input not supported yet!\n");
00844                 return 0;
00845             // FEtk MC Simplex Format (MCSF)
00846             case VDF_MCSF:
00847                 Vnm_tprint( 2, "MCSF input not supported yet!\n");
00848                 return 0;
00849             // AVS UCD format
00850             case VDF_AVS:
00851                 Vnm_tprint( 2, "AVS input not supported yet!\n");
00852                 return 0;
00853             default:
00854                 Vnm_tprint( 2, "Invalid data format (%d)!\n",
00855                             nosh->potfmt[i]);
00856         }
00857     }

```



```

00857         return 0;
00858     }
00859 }
00860
00861     return 1;
00862
00863 }
00864
00865 VPUBLIC void killPotMaps(NOsh *nosh,
00866                         Vgrid *map[NOSH_MAXMOL]
00867                         ) {
00868
00869     int i;
00870
00871     if (nosh->npot > 0) {
00872 #ifndef VAPBSQUIET
00873         Vnm_tprint( 1, "Destroying %d potential maps\n", nosh->npot);
00874 #endif
00875         for (i=0; i<nosh->npot; i++) Vgrid_dtor(&(map[i]));
00876     }
00877     else return;
00878 }
00879
00880
00884 VPUBLIC int loadChargeMaps(NOsh *nosh,
00885                           Vgrid *map[NOSH_MAXMOL]
00886                           ) {
00887
00888     int i,
00889         ii,
00890         len;
00891     double sum;
00892
00893     if (nosh->ncharge > 0)
00894         Vnm_tprint( 1, "Got paths for %d charge maps\n", nosh->ncharge);
00895     else return 1;
00896
00897     for (i=0; i<nosh->ncharge; i++) {
00898         Vnm_tprint( 1, "Reading charge map data from %s:\n",
00899                     nosh->chargepath[i]);
00900         map[i] = Vgrid_ctor(0, 0, 0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, VNULL);
00901
00902         // Determine data format and read data
00903         switch (nosh->chargefmt[i]) {
00904             case VDF_DX:
00905                 if (Vgrid_readDX(map[i], "FILE", "ASC", VNULL,
00906                                nosh->chargepath[i]) != 1) {
00907                     Vnm_tprint( 2, "Fatal error while reading from %s\n",
00908                                 nosh->chargepath[i]);
00909                     return 0;
00910                 }
00911                 Vnm_tprint(1, "  %d x %d x %d grid\n",
00912                             map[i]->nx, map[i]->ny, map[i]->nz);
00913                 Vnm_tprint(1, "    (%g, %g, %g) A spacings\n",
00914                             map[i]->hx, map[i]->hy, map[i]->hz);
00915                 Vnm_tprint(1, "    (%g, %g, %g) A lower corner\n",
00916                             map[i]->xmin, map[i]->ymin, map[i]->zmin);
00917                 sum = 0;
00918                 for (ii=0, len=map[i]->nx*map[i]->ny*map[i]->nz; ii<len; ii++) {
00919                     sum += (map[i]->data[ii]);
00920                 }
00921                 sum = sum*map[i]->hx*map[i]->hy*map[i]->hz;
00922                 Vnm_tprint(1, "  Charge map integral = %3.2e e\n", sum);
00923                 break;
00924             case VDF_DXBIN:
00925                 //TODO: write Vgrid_readDXBIN and possibly change if stmt.
00926                 if (Vgrid_readDXBIN(map[i], "FILE", "ASC", VNULL,
00927                                    nosh->chargepath[i]) != 1) {
00928                     Vnm_tprint( 2, "Fatal error while reading from %s\n",
00929                                 nosh->chargepath[i]);
00930                     return 0;
00931                 }
00932                 Vnm_tprint(1, "  %d x %d x %d grid\n",
00933                             map[i]->nx, map[i]->ny, map[i]->nz);
00934                 Vnm_tprint(1, "    (%g, %g, %g) A spacings\n",
00935                             map[i]->hx, map[i]->hy, map[i]->hz);
00936                 Vnm_tprint(1, "    (%g, %g, %g) A lower corner\n",
00937                             map[i]->xmin, map[i]->ymin, map[i]->zmin);
00938                 sum = 0;
00939                 for (ii=0, len=map[i]->nx*map[i]->ny*map[i]->nz; ii<len; ii++) {
00940                     sum += (map[i]->data[ii]);

```

```

00941     }
00942     sum = sum*map[i]->hx*map[i]->hy*map[i]->hz;
00943     Vnm_tprint(1, " Charge map integral = %3.2e e\n", sum);
00944     break;
00945     case VDF_UHBD:
00946         Vnm_tprint( 2, "UHBD input not supported yet!\n");
00947         return 0;
00948     case VDF_AVS:
00949         Vnm_tprint( 2, "AVS input not supported yet!\n");
00950         return 0;
00951     case VDF_MCSF:
00952         Vnm_tprint(2, "MCSF input not supported yet!\n");
00953         return 0;
00954     case VDF_GZ:
00955         if (Vgrid_readGZ(map[i], nosh->chargepath[i]) != 1) {
00956             Vnm_tprint( 2, "Fatal error while reading from %s\n",
00957                 nosh->chargepath[i]);
00958             return 0;
00959         }
00960         Vnm_tprint(1, " %d x %d x %d grid\n",
00961             map[i]->nx, map[i]->ny, map[i]->nz);
00962         Vnm_tprint(1, " (%g, %g, %g) A spacings\n",
00963             map[i]->hx, map[i]->hy, map[i]->hz);
00964         Vnm_tprint(1, " (%g, %g, %g) A lower corner\n",
00965             map[i]->xmin, map[i]->ymin, map[i]->zmin);
00966         sum = 0;
00967         for (ii=0, len=map[i]->nx*map[i]->ny*map[i]->nz; ii<len; ii++) {
00968             sum += (map[i]->data[ii]);
00969         }
00970         sum = sum*map[i]->hx*map[i]->hy*map[i]->hz;
00971         Vnm_tprint(1, " Charge map integral = %3.2e e\n", sum);
00972         break;
00973     default:
00974         Vnm_tprint( 2, "Invalid data format (%d)!\n",
00975             nosh->kappafmt[i]);
00976         return 0;
00977     }
00978 }
00979
00980 return 1;
00981 }
00982 }
00983
00984 VPUBLIC void killChargeMaps(NOsh *nosh,
00985     Vgrid *map[NOSH_MAXMOL]
00986 ) {
00987
00988     int i;
00989
00990     if (nosh->ncharge > 0) {
00991 #ifndef VAPBSQUIET
00992         Vnm_tprint( 1, "Destroying %d charge maps\n", nosh->ncharge);
00993 #endif
00994         for (i=0; i<nosh->ncharge; i++) Vgrid_dtor(&(map[i]));
00995     }
00996 }
00997
00998 else return;
00999
01000 }
01001
01002 VPUBLIC void printPBEPARM(PBEParm *pbeparm) {
01003
01004     int i;
01005     double ionstr = 0.0;
01006
01007     for (i=0; i<pbeparm->nion; i++)
01008         ionstr += 0.5*(VSQR(pbeparm->ionq[i])*pbeparm->ionc[i]);
01009
01010     Vnm_tprint( 1, " Molecule ID: %d\n", pbeparm->molid);
01011     switch (pbeparm->pbetype) {
01012     case PBE_NPBE:
01013         Vnm_tprint( 1, " Nonlinear traditional PBE\n");
01014         break;
01015     case PBE_LPBE:
01016         Vnm_tprint( 1, " Linearized traditional PBE\n");
01017         break;
01018     case PBE_NRPBE:
01019         Vnm_tprint( 1, " Nonlinear regularized PBE\n");
01020         Vnm_tprint( 2, " ** Sorry, but Nathan broke the nonlinear regularized PBE implementation.
01021             **\n");

```

```

01021         Vnm_tprint( 2, "  ** Please let us know if you are interested in using it. **\n");
01022         VASSERT(0);
01023         break;
01024     case PBE_LRPBE:
01025         Vnm_tprint( 1, "  Linearized regularized PBE\n");
01026         break;
01027     case PBE_SMPBE: /* SMPBE Added */
01028         Vnm_tprint( 1, "  Nonlinear Size-Modified PBE\n");
01029         break;
01030     default:
01031         Vnm_tprint(2, "  Unknown PBE type (%d)!\n", pbeparm->pbetype);
01032         break;
01033     }
01034     if (pbeparm->bcbfl == BCFL_ZERO) {
01035         Vnm_tprint( 1, "  Zero boundary conditions\n");
01036     } else if (pbeparm->bcbfl == BCFL_SDH) {
01037         Vnm_tprint( 1, "  Single Debye-Huckel sphere boundary \
01038 conditions\n");
01039     } else if (pbeparm->bcbfl == BCFL_MDH) {
01040         Vnm_tprint( 1, "  Multiple Debye-Huckel sphere boundary \
01041 conditions\n");
01042     } else if (pbeparm->bcbfl == BCFL_FOCUS) {
01043         Vnm_tprint( 1, "  Boundary conditions from focusing\n");
01044     } else if (pbeparm->bcbfl == BCFL_MAP) {
01045         Vnm_tprint( 1, "  Boundary conditions from potential map\n");
01046     } else if (pbeparm->bcbfl == BCFL_MEM) {
01047         Vnm_tprint( 1, "  Membrane potential boundary conditions.\n");
01048     }
01049     Vnm_tprint( 1, "  %d ion species (%4.3f M ionic strength):\n",
01050         pbeparm->nion, ionstr);
01051     for (i=0; i<pbeparm->nion; i++) {
01052         Vnm_tprint( 1, "    %4.3f A-radius, %4.3f e-charge, \
01053 %4.3f M concentration\n",
01054             pbeparm->ionr[i], pbeparm->ionq[i], pbeparm->ionc[i]);
01055     }
01056
01057     if (pbeparm->pbetype == PBE_SMPBE) { /* SMPBE Added */
01058         Vnm_tprint( 1, "  Lattice spacing: %4.3f A (SMPBE) \n", pbeparm->smvolume);
01059         Vnm_tprint( 1, "  Relative size parameter: %4.3f (SMPBE) \n", pbeparm->smsize);
01060     }
01061
01062     Vnm_tprint( 1, "  Solute dielectric: %4.3f\n", pbeparm->pdie);
01063     Vnm_tprint( 1, "  Solvent dielectric: %4.3f\n", pbeparm->sdie);
01064     switch (pbeparm->srfm) {
01065     case 0:
01066         Vnm_tprint( 1, "  Using \"molecular\" surface \
01067 definition; no smoothing\n");
01068         Vnm_tprint( 1, "  Solvent probe radius: %4.3f A\n",
01069             pbeparm->srad);
01070         break;
01071     case 1:
01072         Vnm_tprint( 1, "  Using \"molecular\" surface definition;\
01073 harmonic average smoothing\n");
01074         Vnm_tprint( 1, "  Solvent probe radius: %4.3f A\n",
01075             pbeparm->srad);
01076         break;
01077     case 2:
01078         Vnm_tprint( 1, "  Using spline-based surface definition;\
01079 window = %4.3f\n", pbeparm->swin);
01080         break;
01081     default:
01082         break;
01083     }
01084     Vnm_tprint( 1, "  Temperature: %4.3f K\n", pbeparm->temp);
01085     if (pbeparm->calcenergy != PCE_NO) Vnm_tprint( 1, "  Electrostatic \
01086 energies will be calculated\n");
01087     if (pbeparm->calcforce == PCF_TOTAL) Vnm_tprint( 1, "  Net solvent \
01088 forces will be calculated\n");
01089     if (pbeparm->calcforce == PCF_COMPS) Vnm_tprint( 1, "  All-atom \
01090 solvent forces will be calculated\n");
01091     for (i=0; i<pbeparm->numwrite; i++) {
01092         switch (pbeparm->writetype[i]) {
01093         case VDT_CHARGE:
01094             Vnm_tprint(1, "  Charge distribution to be written to ");
01095             break;
01096         case VDT_POT:
01097             Vnm_tprint(1, "  Potential to be written to ");
01098             break;
01099         case VDT_SMOL:
01100             Vnm_tprint(1, "  Molecular solvent accessibility \
01101 to be written to ");

```

```

01102         break;
01103     case VDT_SSPL:
01104         Vnm_tprint(1, " Spline-based solvent accessibility \
01105 to be written to ");
01106         break;
01107     case VDT_VDW:
01108         Vnm_tprint(1, " van der Waals solvent accessibility \
01109 to be written to ");
01110         break;
01111     case VDT_IVDW:
01112         Vnm_tprint(1, " Ion accessibility to be written to ");
01113         break;
01114     case VDT_LAP:
01115         Vnm_tprint(1, " Potential Laplacian to be written to ");
01116         break;
01117     case VDT_EDENS:
01118         Vnm_tprint(1, " Energy density to be written to ");
01119         break;
01120     case VDT_NDENS:
01121         Vnm_tprint(1, " Ion number density to be written to ");
01122         break;
01123     case VDT_QDENS:
01124         Vnm_tprint(1, " Ion charge density to be written to ");
01125         break;
01126     case VDT_DIELX:
01127         Vnm_tprint(1, " X-shifted dielectric map to be written \
01128 to ");
01129         break;
01130     case VDT_DIELY:
01131         Vnm_tprint(1, " Y-shifted dielectric map to be written \
01132 to ");
01133         break;
01134     case VDT_DIELZ:
01135         Vnm_tprint(1, " Z-shifted dielectric map to be written \
01136 to ");
01137         break;
01138     case VDT_KAPPA:
01139         Vnm_tprint(1, " Kappa map to be written to ");
01140         break;
01141     case VDT_ATOMPOT:
01142         Vnm_tprint(1, " Atom potentials to be written to ");
01143         break;
01144     default:
01145         Vnm_tprint(2, " Invalid data type for writing!\n");
01146         break;
01147 }
01148 switch (pbeparm->writefmt[i]) {
01149     case VDF_DX:
01150         Vnm_tprint(1, "%s.%s\n", pbeparm->writestem[i], "dx");
01151         break;
01152     case VDF_DXBIN:
01153         Vnm_tprint(1, "%s.%s\n", pbeparm->writestem[i], "dxbin");
01154         break;
01155     case VDF_GZ:
01156         Vnm_tprint(1, "%s.%s\n", pbeparm->writestem[i], "dx.gz");
01157         break;
01158     case VDF_UHBD:
01159         Vnm_tprint(1, "%s.%s\n", pbeparm->writestem[i], "grd");
01160         break;
01161     case VDF_AVS:
01162         Vnm_tprint(1, "%s.%s\n", pbeparm->writestem[i], "ucd");
01163         break;
01164     case VDF_MCSF:
01165         Vnm_tprint(1, "%s.%s\n", pbeparm->writestem[i], "mcsf");
01166         break;
01167     case VDF_FLAT:
01168         Vnm_tprint(1, "%s.%s\n", pbeparm->writestem[i], "txt");
01169         break;
01170     default:
01171         Vnm_tprint(2, " Invalid format for writing!\n");
01172         break;
01173 }
01174 }
01175 }
01176 }
01177 }
01178
01179 VPUBLIC void printMGPARM(MGparm *mgparm, double realCenter[3]) {
01180
01181     switch (mgparm->chgm) {
01182         case 0:

```

```

01183         Vnm_tprint(1, " Using linear spline charge discretization.\n");
01184         break;
01185     case 1:
01186         Vnm_tprint(1, " Using cubic spline charge discretization.\n");
01187         break;
01188     default:
01189         break;
01190 }
01191 if (mgparm->type == MCT_PARALLEL) {
01192     Vnm_tprint(1, " Partition overlap fraction = %g\n",
01193         mgparm->ofrac);
01194     Vnm_tprint(1, " Processor array = %d x %d x %d\n",
01195         mgparm->pdime[0], mgparm->pdime[1], mgparm->pdime[2]);
01196 }
01197 Vnm_tprint(1, " Grid dimensions: %d x %d x %d\n",
01198     mgparm->dime[0], mgparm->dime[1], mgparm->dime[2]);
01199 Vnm_tprint(1, " Grid spacings: %4.3f x %4.3f x %4.3f\n",
01200     mgparm->grid[0], mgparm->grid[1], mgparm->grid[2]);
01201 Vnm_tprint(1, " Grid lengths: %4.3f x %4.3f x %4.3f\n",
01202     mgparm->glen[0], mgparm->glen[1], mgparm->glen[2]);
01203 Vnm_tprint(1, " Grid center: (%4.3f, %4.3f, %4.3f)\n",
01204     realCenter[0], realCenter[1], realCenter[2]);
01205 Vnm_tprint(1, " Multigrid levels: %d\n", mgparm->nlev);
01206
01207 }
01208
01212 VPUBLIC int initMG(int icalc,
01213     NOSH *nosh, MGparm *mgparm,
01214     PBEparm *pbeparm,
01215     double realCenter[3],
01216     Vpbe *pbe[NOSH_MAXCALC],
01217     Valist *alist[NOSH_MAXMOL],
01218     Vgrid *dielXMap[NOSH_MAXMOL],
01219     Vgrid *dielYMap[NOSH_MAXMOL],
01220     Vgrid *dielZMap[NOSH_MAXMOL],
01221     Vgrid *kappaMap[NOSH_MAXMOL],
01222     Vgrid *chargeMap[NOSH_MAXMOL],
01223     Vpmgp *pmgp[NOSH_MAXCALC],
01224     Vpmg *pmg[NOSH_MAXCALC],
01225     Vgrid *potMap[NOSH_MAXMOL]
01226 ) {
01227
01228     int j,
01229         focusFlag,
01230         iatom;
01231     size_t bytesTotal,
01232         highWater;
01233     double sparm,
01234         iparm,
01235         q;
01236     Vatom *atom = VNULL;
01237     Vgrid *theDielXMap = VNULL,
01238         *theDielYMap = VNULL,
01239         *theDielZMap = VNULL;
01240     Vgrid *theKappaMap = VNULL,
01241         *thePotMap = VNULL,
01242         *theChargeMap = VNULL;
01243     Valist *myalist = VNULL;
01244
01245     Vnm_tstart(APBS_TIMER_SETUP, "Setup timer");
01246
01247     /* Update the grid center */
01248     for (j=0; j<3; j++) realCenter[j] = mgparm->center[j];
01249
01250     /* Check for completely-neutral molecule */
01251     q = 0;
01252     myalist = alist[pbeparm->molid-1];
01253     for (iatom=0; iatom<Valist_getNumberAtoms(myalist); iatom++) {
01254         atom = Valist_getAtom(myalist, iatom);
01255         q += VSQR(Vatom_getCharge(atom));
01256     }
01257     /* D. Gohara 10/22/09 - disabled
01258     if (q < (1e-6)) {
01259         Vnm_tprint(2, "Molecule #d is uncharged!\n", pbeparm->molid);
01260         Vnm_tprint(2, "Sum square charge = %g!\n", q);
01261         return 0;
01262     }
01263     */
01264
01265     /* Set up PBE object */
01266     Vnm_tprint(0, "Setting up PBE object...\n");

```

```

01267     if (pbeparm->srfm == VSM_SPLINE) {
01268         sparm = pbeparm->swin;
01269     } else {
01270         sparm = pbeparm->srad;
01271     }
01272     if (pbeparm->nion > 0) {
01273         iparm = pbeparm->ionr[0];
01274     } else {
01275         iparm = 0.0;
01276     }
01277     if (pbeparm->bcbfl == BCFL_FOCUS) {
01278         if (icalc == 0) {
01279             Vnm_tprint( 2, "Can't focus first calculation!\n");
01280             return 0;
01281         }
01282         focusFlag = 1;
01283     } else {
01284         focusFlag = 0;
01285     }
01286
01287     // Construct Vpbe object
01288     pbe[icalc] = Vpbe_ctor(myalist, pbeparm->nion,
01289                          pbeparm->ionc, pbeparm->ionr, pbeparm->ionq,
01290                          pbeparm->temp, pbeparm->pdie,
01291                          pbeparm->sdie, sparm, focusFlag, pbeparm->sdens,
01292                          pbeparm->zmem, pbeparm->Lmem, pbeparm->mdie,
01293                          pbeparm->memv);
01294
01295     /* Set up PDE object */
01296     Vnm_tprint(0, "Setting up PDE object...\n");
01297     switch (pbeparm->pbetype) {
01298     case PBE_NPBE:
01299         /* TEMPORARY USEAQUA */
01300         mgparm->nonlntype = NONLIN_NPBE;
01301         mgparm->method = (mgparm->useAqua == 1) ? VSOL_NewtonAqua : VSOL_Newton;
01302         pmgp[icalc] = Vpmgp_ctor(mgparm);
01303         break;
01304     case PBE_LPBE:
01305         /* TEMPORARY USEAQUA */
01306         mgparm->nonlntype = NONLIN_LPBE;
01307         mgparm->method = (mgparm->useAqua == 1) ? VSOL_CGMGAqua : VSOL_MG;
01308         pmgp[icalc] = Vpmgp_ctor(mgparm);
01309         break;
01310     case PBE_LRPBE:
01311         Vnm_tprint(2, "Sorry, LRPBE isn't supported with the MG solver!\n");
01312         return 0;
01313     case PBE_NRPBE:
01314         Vnm_tprint(2, "Sorry, NRPBE isn't supported with the MG solver!\n");
01315         return 0;
01316     case PBE_SMPBE: /* SMPBE Added */
01317         /* Due to numerical issues the SMPBE is currently disabled. (JMB)*/
01318         Vnm_tprint(2, " ** Sorry, due to numerical stability issues SMPBE is currently disabled. We
01319 apologize for the inconvenience.\n");
01320         Vnm_tprint(2, " ** Please let us know if you would like to use it in the future.\n");
01321         return 0;
01322
01323         /*
01324         mgparm->nonlntype = NONLIN_SMPBE;
01325         pmgp[icalc] = Vpmgp_ctor(mgparm);
01326         */
01327         /* Copy Code */
01328         /*
01329         pbe[icalc]->smsize = pbeparm->smsize;
01330         pbe[icalc]->smvolume = pbeparm->smvolume;
01331         pbe[icalc]->ipkey = pmgp[icalc]->ipkey;
01332         break;
01333         */
01334     default:
01335         Vnm_tprint(2, "Error! Unknown PBE type (%d)!\n", pbeparm->pbetype);
01336         return 0;
01337     }
01338     Vnm_tprint(0, "Setting PDE center to local center...\n");
01339     pmgp[icalc]->bcbfl = pbeparm->bcbfl;
01340     pmgp[icalc]->xcen = realCenter[0];
01341     pmgp[icalc]->ycen = realCenter[1];
01342     pmgp[icalc]->zcen = realCenter[2];
01343
01344     if (pbeparm->bcbfl == BCFL_FOCUS) {
01345         if (icalc == 0) {
01346             Vnm_tprint( 2, "Can't focus first calculation!\n");

```

```

01347         return 0;
01348     }
01349     /* Focusing requires the previous calculation in order to setup the
01350     current run... */
01351     pmg[icalc] = Vpmg_ctor(pmgp[icalc], pbe[icalc], 1, pmg[icalc-1],
01352                          mgparm, pbeparm->calcenergy);
01353     /* ...however, it should be done with the previous calculation now, so
01354     we should be able to destroy it here. */
01355     /* Vpmg_dtor(&(pmg[icalc-1])); */
01356 } else {
01357     if (icalc>0) Vpmg_dtor(&(pmg[icalc-1]));
01358     pmg[icalc] = Vpmg_ctor(pmgp[icalc], pbe[icalc], 0, VNULL, mgparm, PCE_NO);
01359 }
01360 if (icalc>0) {
01361     Vpmgp_dtor(&(pmgp[icalc-1]));
01362     Vpbe_dtor(&(pbe[icalc-1]));
01363 }
01364 if (pbeparm->useDielMap) {
01365     if ((pbeparm->dielMapID-1) < nosh->ndiel) {
01366         theDielXMap = dielXMap[pbeparm->dielMapID-1];
01367     } else {
01368         Vnm_print(2, "Error! %d is not a valid dielectric map ID!\n",
01369                  pbeparm->dielMapID);
01370         return 0;
01371     }
01372 }
01373 if (pbeparm->useDielMap) {
01374     if ((pbeparm->dielMapID-1) < nosh->ndiel) {
01375         theDielYMap = dielYMap[pbeparm->dielMapID-1];
01376     } else {
01377         Vnm_print(2, "Error! %d is not a valid dielectric map ID!\n",
01378                  pbeparm->dielMapID);
01379         return 0;
01380     }
01381 }
01382 if (pbeparm->useDielMap) {
01383     if ((pbeparm->dielMapID-1) < nosh->ndiel) {
01384         theDielZMap = dielZMap[pbeparm->dielMapID-1];
01385     } else {
01386         Vnm_print(2, "Error! %d is not a valid dielectric map ID!\n",
01387                  pbeparm->dielMapID);
01388         return 0;
01389     }
01390 }
01391 if (pbeparm->useKappaMap) {
01392     if ((pbeparm->kappaMapID-1) < nosh->nkappa) {
01393         theKappaMap = kappaMap[pbeparm->kappaMapID-1];
01394     } else {
01395         Vnm_print(2, "Error! %d is not a valid kappa map ID!\n",
01396                  pbeparm->kappaMapID);
01397         return 0;
01398     }
01399 }
01400 if (pbeparm->usePotMap) {
01401     if ((pbeparm->potMapID-1) < nosh->npot) {
01402         thePotMap = potMap[pbeparm->potMapID-1];
01403     } else {
01404         Vnm_print(2, "Error! %d is not a valid potential map ID!\n",
01405                  pbeparm->potMapID);
01406         return 0;
01407     }
01408 }
01409 if (pbeparm->useChargeMap) {
01410     if ((pbeparm->chargeMapID-1) < nosh->ncharge) {
01411         theChargeMap = chargeMap[pbeparm->chargeMapID-1];
01412     } else {
01413         Vnm_print(2, "Error! %d is not a valid charge map ID!\n",
01414                  pbeparm->chargeMapID);
01415         return 0;
01416     }
01417 }
01418
01419 if (pbeparm->bconf == BCFL_MAP && thePotMap == VNULL) {
01420     Vnm_print(2, "Warning: You specified 'bconf map' in the input file, but no potential map was
found.\n");
01421     Vnm_print(2, "          You must specify 'usemap pot' statement in the APBS input file!\n");
01422     Vnm_print(2, "Bailing out ...\n");
01423     return 0;
01424 }
01425
01426 // Initialize calculation coefficients

```

```

01427     if (!Vpmg_fillco(pmg[icalc],
01428                     pbeparm->srfm, pbeparm->swin, mgparm->chgm,
01429                     pbeparm->useDielMap, theDielXMap,
01430                     pbeparm->useDielMap, theDielYMap,
01431                     pbeparm->useDielMap, theDielZMap,
01432                     pbeparm->useKappaMap, theKappaMap,
01433                     pbeparm->usePotMap, thePotMap,
01434                     pbeparm->useChargeMap, theChargeMap)) {
01435         Vnm_print(2, "initMG: problems setting up coefficients (fillco)!\n");
01436         return 0;
01437     }
01438
01439     /* Print a few derived parameters */
01440 #ifndef VAPBSQUIET
01441     Vnm_tprint(1, " Debye length: %g A\n", Vpbe_getDeblen(pbe[icalc]));
01442 #endif
01443
01444     /* Setup time statistics */
01445     Vnm_tstop(APBS_TIMER_SETUP, "Setup timer");
01446
01447     /* Memory statistics */
01448     bytesTotal = Vmem_bytesTotal();
01449     highWater = Vmem_highWaterTotal();
01450
01451 #ifndef VAPBSQUIET
01452     Vnm_tprint(1, " Current memory usage: %4.3f MB total, \
01453 %4.3f MB high water\n", (double)(bytesTotal)/(1024.*1024.),
01454                     (double)(highWater)/(1024.*1024.));
01455 #endif
01456
01457     return 1;
01458 }
01459
01460
01461 VPUBLIC void killMG(NOsh *nosh, Vpbe *pbe[NOSH_MAXCALC],
01462                  Vpmgp *pmgp[NOSH_MAXCALC], Vpmg *pmg[NOSH_MAXCALC]) {
01463
01464     int i;
01465
01466 #ifndef VAPBSQUIET
01467     Vnm_tprint(1, "Destroying multigrid structures.\n");
01468 #endif
01469
01470     /*
01471      There appears to be a relationship (or this is a bug in Linux, can't tell
01472      at the moment, since Linux is the only OS that seems to be affected)
01473      between one of the three object types: Vpbe, Vpmg or Vpmgp that requires
01474      deallocations to be performed in a specific order. This results in a
01475      bug some of the time when freeing Vpmg objects below. Therefore it
01476      appears to be important to release the Vpmg structs BEFORE the Vpmgp structs .
01477     */
01478     Vpmg_dtor(&(pmg[nosh->ncalc-1]));
01479
01480     for(i=0; i<nosh->ncalc; i++){
01481         Vpbe_dtor(&(pbe[i]));
01482         Vpmgp_dtor(&(pmgp[i]));
01483     }
01484 }
01485
01486
01487 VPUBLIC int solveMG(NOsh *nosh,
01488                  Vpmg *pmg,
01489                  MGparm_CalcType type
01490                  ) {
01491
01492     int nx,
01493         ny,
01494         nz,
01495         i;
01496
01497     if (nosh != VNULL) {
01498         if (nosh->bogus) return 1;
01499     }
01500
01501     Vnm_tstart(APBS_TIMER_SOLVER, "Solver timer");
01502
01503
01504     if (type != MCT_DUMMY) {
01505         if (!Vpmg_solve(pmg)) {
01506             Vnm_print(2, " Error during PDE solution!\n");
01507             return 0;

```



```

01508     }
01509   } else {
01510     Vnm_tprint( 1, " Skipping solve for mg-dummy run; zeroing \
01511 solution array\n");
01512     nx = pmg->pmgp->nx;
01513     ny = pmg->pmgp->ny;
01514     nz = pmg->pmgp->nz;
01515     for (i=0; i<nx*ny*nz; i++) pmg->u[i] = 0.0;
01516   }
01517   Vnm_tstop(APBS_TIMER_SOLVER, "Solver timer");
01518
01519   return 1;
01520 }
01521 }
01522
01523 VPUBLIC int setPartMG(NOsh *nosh,
01524                     MGparm *mgparm,
01525                     Vpmg *pmg
01526 ) {
01527
01528   int j;
01529   double partMin[3],
01530         partMax[3];
01531
01532   if (nosh->bogus) return 1;
01533
01534   if (mgparm->type == MCT_PARALLEL) {
01535     for (j=0; j<3; j++) {
01536       partMin[j] = mgparm->partDisjCenter[j] - 0.5*mgparm->partDisjLength[j];
01537       partMax[j] = mgparm->partDisjCenter[j] + 0.5*mgparm->partDisjLength[j];
01538     }
01539     #if 0
01540     Vnm_tprint(1, "setPartMG (%s, %d): Disj part center = (%g, %g, %g)\n",
01541               __FILE__, __LINE__,
01542               mgparm->partDisjCenter[0],
01543               mgparm->partDisjCenter[1],
01544               mgparm->partDisjCenter[2]
01545             );
01546     Vnm_tprint(1, "setPartMG (%s, %d): Disj part lower corner = (%g, %g, %g)\n",
01547               __FILE__, __LINE__, partMin[0], partMin[1], partMin[2]);
01548     Vnm_tprint(1, "setPartMG (%s, %d): Disj part upper corner = (%g, %g, %g)\n",
01549               __FILE__, __LINE__,
01550               partMax[0], partMax[1], partMax[2]);
01551     #endif
01552   } else {
01553     for (j=0; j<3; j++) {
01554       partMin[j] = mgparm->center[j] - 0.5*mgparm->glen[j];
01555       partMax[j] = mgparm->center[j] + 0.5*mgparm->glen[j];
01556     }
01557   }
01558   /* Vnm_print(1, "DEBUG (%s, %d): setPartMG calling setPart with upper corner \
01559 %g %g %g and lower corner %g %g %g\n", __FILE__, __LINE__,
01560               partMin[0], partMin[1], partMin[2],
01561               partMax[0], partMax[1], partMax[2]); */
01562   Vpmg_setPart(pmg, partMin, partMax, mgparm->partDisjOwnSide);
01563
01564
01565   return 1;
01566 }
01567 }
01568
01569 VPUBLIC int energyMG(NOsh *nosh,
01570                    int icalc,
01571                    Vpmg *pmg,
01572                    int *nenergy,
01573                    double *totEnergy,
01574                    double *qfEnergy,
01575                    double *qmEnergy,
01576                    double *dielEnergy
01577 ) {
01578
01579   Valist *alist;
01580   Vatom *atom;
01581   int i,
01582       extEnergy;
01583   double tenergy;
01584   MGparm *mgparm;
01585   PBEParm *pbeparm;
01586
01587   mgparm = nosh->calc[icalc]->mgparm;
01588   pbeparm = nosh->calc[icalc]->pbeparm;

```

```

01589
01590     Vnm_tstart(APBS_TIMER_ENERGY, "Energy timer");
01591     extEnergy = 1;
01592
01593     if (pbeparm->calcenergy == PCE_TOTAL) {
01594         *nenergy = 1;
01595         /* Some processors don't count */
01596         if (nosh->bogus == 0) {
01597             *totEnergy = Vpmg_energy(pmg, extEnergy);
01598 #ifndef VAPBSQUIET
01599             Vnm_tprint( 1, " Total electrostatic energy = %1.12E kJ/mol\n",
01600                 Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na*(totEnergy));
01601 #endif
01602         } else *totEnergy = 0;
01603     } else if (pbeparm->calcenergy == PCE_COMPS) {
01604         *nenergy = 1;
01605         *totEnergy = Vpmg_energy(pmg, extEnergy);
01606         *qfEnergy = Vpmg_qfEnergy(pmg, extEnergy);
01607         *qmEnergy = Vpmg_qmEnergy(pmg, extEnergy);
01608         *dielEnergy = Vpmg_dielEnergy(pmg, extEnergy);
01609 #ifndef VAPBSQUIET
01610         Vnm_tprint( 1, " Total electrostatic energy = %1.12E \
01611 kJ/mol\n", Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na*(totEnergy));
01612         Vnm_tprint( 1, " Fixed charge energy = %g kJ/mol\n",
01613             0.5*Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na*(qfEnergy));
01614         Vnm_tprint( 1, " Mobile charge energy = %g kJ/mol\n",
01615             Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na*(qmEnergy));
01616         Vnm_tprint( 1, " Dielectric energy = %g kJ/mol\n",
01617             Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na*(dielEnergy));
01618         Vnm_tprint( 1, " Per-atom energies:\n");
01619 #endif
01620         alist = pmg->pbe->alist;
01621         for (i=0; i<Valist_getNumberAtoms(alist); i++) {
01622             atom = Valist_getAtom(alist, i);
01623             tenergy = Vpmg_qfAtomEnergy(pmg, atom);
01624 #ifndef VAPBSQUIET
01625             Vnm_tprint( 1, " Atom %d: %1.12E kJ/mol\n", i,
01626                 0.5*Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na*tenergy);
01627 #endif
01628         }
01629     } else *nenergy = 0;
01630
01631     Vnm_tstop(APBS_TIMER_ENERGY, "Energy timer");
01632
01633     return 1;
01634 }
01635
01636 VPUBLIC int forceMG(Vmem *mem,
01637     NOSH *nosh,
01638     PBeparm *pbeparm,
01639     MGparm *mgparm,
01640     Vpmg *pmg,
01641     int *nforce,
01642     AtomForce **atomForce,
01643     Valist *alist[NOSH_MAXMOL]
01644 ) {
01645
01646     int j,
01647         k;
01648     double qfForce[3],
01649         dbForce[3],
01650         ibForce[3];
01651
01652     Vnm_tstart(APBS_TIMER_FORCE, "Force timer");
01653
01654 #ifndef VAPBSQUIET
01655     Vnm_tprint( 1, " Calculating forces...\n");
01656 #endif
01657
01658     if (pbeparm->calcforce == PCF_TOTAL) {
01659         *nforce = 1;
01660         *atomForce = (AtomForce *)Vmem_malloc(mem, 1, sizeof(AtomForce));
01661         /* Clear out force arrays */
01662         for (j=0; j<3; j++) {
01663             (*atomForce)[0].qfForce[j] = 0;
01664             (*atomForce)[0].ibForce[j] = 0;
01665             (*atomForce)[0].dbForce[j] = 0;
01666         }
01667         for (j=0; j<Valist_getNumberAtoms(alist[pbeparm->molid-1]); j++) {
01668             if (nosh->bogus == 0) {
01669                 VASSERT(Vpmg_qfForce(pmg, qfForce, j, mgparm->chgm));

```

```

01670         VASSERT(Vpmg_ibForce(pmg, ibForce, j, pbeparm->srfm));
01671         VASSERT(Vpmg_dbForce(pmg, dbForce, j, pbeparm->srfm));
01672     } else {
01673         for (k=0; k<3; k++) {
01674             qfForce[k] = 0;
01675             ibForce[k] = 0;
01676             dbForce[k] = 0;
01677         }
01678     }
01679     for (k=0; k<3; k++) {
01680         (*atomForce)[0].qfForce[k] += qfForce[k];
01681         (*atomForce)[0].ibForce[k] += ibForce[k];
01682         (*atomForce)[0].dbForce[k] += dbForce[k];
01683     }
01684 }
01685 #ifndef VAPBSQUIET
01686 Vnm_tprint( 1, " Printing net forces for molecule %d (kJ/mol/A)\n",
01687             pbeparm->molid);
01688 Vnm_tprint( 1, " Legend:\n");
01689 Vnm_tprint( 1, " qf -- fixed charge force\n");
01690 Vnm_tprint( 1, " db -- dielectric boundary force\n");
01691 Vnm_tprint( 1, " ib -- ionic boundary force\n");
01692 Vnm_tprint( 1, " qf %4.3e %4.3e %4.3e\n",
01693             Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na*(atomForce)[0].qfForce[0],
01694             Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na*(atomForce)[0].qfForce[1],
01695             Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na*(atomForce)[0].qfForce[2]);
01696 Vnm_tprint( 1, " ib %4.3e %4.3e %4.3e\n",
01697             Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na*(atomForce)[0].ibForce[0],
01698             Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na*(atomForce)[0].ibForce[1],
01699             Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na*(atomForce)[0].ibForce[2]);
01700 Vnm_tprint( 1, " db %4.3e %4.3e %4.3e\n",
01701             Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na*(atomForce)[0].dbForce[0],
01702             Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na*(atomForce)[0].dbForce[1],
01703             Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na*(atomForce)[0].dbForce[2]);
01704 #endif
01705 } else if (pbeparm->calcforce == PCF_COMPS) {
01706     *nforce = Valist_getNumberAtoms(alist[pbeparm->molid-1]);
01707     *atomForce = (AtomForce *)Vmem_malloc(mem, *nforce,
01708                                           sizeof(AtomForce));
01709 #ifndef VAPBSQUIET
01710 Vnm_tprint( 1, " Printing per-atom forces for molecule %d (kJ/mol/A)\n",
01711             pbeparm->molid);
01712 Vnm_tprint( 1, " Legend:\n");
01713 Vnm_tprint( 1, " tot n -- total force for atom n\n");
01714 Vnm_tprint( 1, " qf n -- fixed charge force for atom n\n");
01715 Vnm_tprint( 1, " db n -- dielectric boundary force for atom n\n");
01716 Vnm_tprint( 1, " ib n -- ionic boundary force for atom n\n");
01717 #endif
01718 for (j=0; j<Valist_getNumberAtoms(alist[pbeparm->molid-1]); j++) {
01719     if (nosh->bogus == 0) {
01720         VASSERT(Vpmg_qfForce(pmg, (*atomForce)[j].qfForce, j,
01721                             mgparm->chgm));
01722         VASSERT(Vpmg_ibForce(pmg, (*atomForce)[j].ibForce, j,
01723                             pbeparm->srfm));
01724         VASSERT(Vpmg_dbForce(pmg, (*atomForce)[j].dbForce, j,
01725                             pbeparm->srfm));
01726     } else {
01727         for (k=0; k<3; k++) {
01728             (*atomForce)[j].qfForce[k] = 0;
01729             (*atomForce)[j].ibForce[k] = 0;
01730             (*atomForce)[j].dbForce[k] = 0;
01731         }
01732     }
01733 #ifndef VAPBSQUIET
01734 Vnm_tprint( 1, "mgF tot %d %4.3e %4.3e %4.3e\n", j,
01735             Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na \
01736             *((atomForce)[j].qfForce[0]+(*atomForce)[j].ibForce[0]+
01737             (*atomForce)[j].dbForce[0]),
01738             Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na \
01739             *((atomForce)[j].qfForce[1]+(*atomForce)[j].ibForce[1]+
01740             (*atomForce)[j].dbForce[1]),
01741             Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na \
01742             *((atomForce)[j].qfForce[2]+(*atomForce)[j].ibForce[2]+
01743             (*atomForce)[j].dbForce[2]));
01744 Vnm_tprint( 1, "mgF qf %d %4.3e %4.3e %4.3e\n", j,
01745             Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na \
01746             *((atomForce)[j].qfForce[0],
01747             Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na \
01748             *((atomForce)[j].qfForce[1],
01749             Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na \
01750             *((atomForce)[j].qfForce[2]);

```

```

01751         Vnm_tprint( 1, "mgF ib %d %4.3e %4.3e %4.3e\n", j,
01752                     Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na \
01753                     *(*atomForce)[j].ibForce[0],
01754                     Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na \
01755                     *(*atomForce)[j].ibForce[1],
01756                     Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na \
01757                     *(*atomForce)[j].ibForce[2]);
01758         Vnm_tprint( 1, "mgF db %d %4.3e %4.3e %4.3e\n", j,
01759                     Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na \
01760                     *(*atomForce)[j].dbForce[0],
01761                     Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na \
01762                     *(*atomForce)[j].dbForce[1],
01763                     Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na \
01764                     *(*atomForce)[j].dbForce[2]);
01765     #endif
01766     }
01767     } else *nforce = 0;
01768
01769     Vnm_tstop(APBS_TIMER_FORCE, "Force timer");
01770
01771     return 1;
01772 }
01773
01774 VPUBLIC void killEnergy() {
01775
01776     #ifndef VAPBSQUIET
01777         Vnm_tprint(1, "No energy arrays to destroy.\n");
01778     #endif
01779 }
01780
01781 VPUBLIC void killForce(Vmem *mem, Nosh *nosh, int nforce[NOSH_MAXCALC],
01782                      AtomForce *atomForce[NOSH_MAXCALC]) {
01783
01784     int i;
01785
01786     #ifndef VAPBSQUIET
01787         Vnm_tprint(1, "Destroying force arrays.\n");
01788     #endif
01789
01790     for (i=0; i<nosh->ncalc; i++) {
01791
01792         if (nforce[i] > 0) Vmem_free(mem, nforce[i], sizeof(AtomForce),
01793                                     (void **)&(atomForce[i]));
01794     }
01795 }
01796
01797
01798 VPUBLIC int writematMG(int rank, Nosh *nosh, PBeparm *pbeparm, Vpmg *pmg) {
01799
01800     char writematstem[VMAX_ARGLEN];
01801     char outpath[VMAX_ARGLEN];
01802     char mxtype[3];
01803     int strlenmax;
01804
01805     if (nosh->bogus) return 1;
01806
01807     #ifdef HAVE_MPI_H
01808         strlenmax = VMAX_ARGLEN-14;
01809         if ((int)strlen(pbeparm->writematstem) > strlenmax) {
01810             Vnm_tprint(2, " Matrix name (%s) too long (%d char max)!\n",
01811                         pbeparm->writematstem, strlenmax);
01812             Vnm_tprint(2, " Not writing matrix!\n");
01813             return 0;
01814         }
01815         sprintf(writematstem, "%s-PE%d", pbeparm->writematstem, rank);
01816     #else
01817         strlenmax = (int)(VMAX_ARGLEN)-1;
01818         if ((int)strlen(pbeparm->writematstem) > strlenmax) {
01819             Vnm_tprint(2, " Matrix name (%s) too long (%d char max)!\n",
01820                         pbeparm->writematstem, strlenmax);
01821             Vnm_tprint(2, " Not writing matrix!\n");
01822             return 0;
01823         }
01824         if(nosh->ispara == 1){
01825             sprintf(writematstem, "%s-PE%d", pbeparm->writematstem, nosh->proc_rank);
01826         }else{
01827             sprintf(writematstem, "%s", pbeparm->writematstem);
01828         }
01829     #endif
01830
01831

```

```

01832     if (pbeparm->writemat == 1) {
01833         strlenmax = VMAX_ARGLEN-5;
01834         if ((int)strlen(pbeparm->writematstem) > strlenmax) {
01835             Vnm_tprint(2, " Matrix name (%s) too long (%d char max)!\n",
01836                 pbeparm->writematstem, strlenmax);
01837             Vnm_tprint(2, " Not writing matrix!\n");
01838             return 0;
01839         }
01840         sprintf(outpath, "%s.%s", writematstem, "mat");
01841         mxtype[0] = 'R';
01842         mxtype[1] = 'S';
01843         mxtype[2] = 'A';
01844         /* Poisson operator only */
01845         if (pbeparm->writematflag == 0) {
01846             Vnm_tprint(1, " Writing Poisson operator matrix \
01847 to %s...\n", outpath);
01848             /* Linearization of Poisson-Boltzmann operator around solution */
01849         } else if (pbeparm->writematflag == 1) {
01850             Vnm_tprint(1, " Writing linearization of full \
01851 Poisson-Boltzmann operator matrix to %s...\n", outpath);
01852         } else {
01853             Vnm_tprint(2, " Bogus matrix specification\
01854 (%d)!\n", pbeparm->writematflag);
01855             return 0;
01856         }
01857         Vnm_tprint(0, " Printing operator...\n");
01858         //Vpmg_printColComp(pmg, outpath, outpath, mxtype,
01859             // pbeparm->writematflag);
01860         return 0;
01861     }
01862     return 1;
01863 }
01864
01865 VPUBLIC void storeAtomEnergy(Vpmg *pmg, int icalc, double **atomEnergy,
01866     int *nenergy){
01867     Vatom *atom;
01868     Valist *alist;
01869     int i;
01870
01871     alist = pmg->pbe->alist;
01872     *nenergy = Valist_getNumberAtoms(alist);
01873     *atomEnergy = (double *)Vmem_malloc(pmg->vmem, *nenergy, sizeof(double));
01874
01875     for (i=0; i<*nenergy; i++) {
01876         atom = Valist_getAtom(alist, i);
01877         (*atomEnergy)[i] = Vpmg_qfAtomEnergy(pmg, atom);
01878     }
01879 }
01880
01881 VPUBLIC int writedataFlat(
01882     Nosh *nosh,
01883     Vcom *com,
01884     const char *fname,
01885     double totEnergy[NOSH_MAXCALC],
01886     double qfEnergy[NOSH_MAXCALC],
01887     double qmEnergy[NOSH_MAXCALC],
01888     double dielEnergy[NOSH_MAXCALC],
01889     int nenergy[NOSH_MAXCALC],
01890     double *atomEnergy[NOSH_MAXCALC],
01891     int nforce[NOSH_MAXCALC],
01892     AtomForce *atomForce[NOSH_MAXCALC]) {
01893     FILE *file;
01894     time_t now;
01895     int ielec, icalc, i, j;
01896     char *timestring = VNULL;
01897     PBeparm *pbeparm = VNULL;
01898     MGparm *mgparm = VNULL;
01899     double conversion, ltenergy, gtenergy, scalar;
01900
01901     if (nosh->bogus) return 1;
01902
01903     /* Initialize some variables */
01904
01905     icalc = 0;

```

```

01913
01914     file = fopen(fname, "w");
01915     if (file == VNULL) {
01916         Vnm_print(2, "writedataFlat: Problem opening virtual socket %s\n",
01917                 fname);
01918         return 0;
01919     }
01920
01921     /* Strip the newline character from the date */
01922
01923     now = time(VNULL);
01924     timestring = ctime(&now);
01925     fprintf(file, "%s\n", timestring);
01926
01927     for (ielec=0; ielec<nosh->nelec;ielec++) { /* elec loop */
01928
01929         /* Initialize per-elec pointers */
01930
01931         mgparm = nosh->calc[icalc]->mgparm;
01932         pbeparm = nosh->calc[icalc]->pbeparm;
01933
01934         /* Convert from kT/e to kJ/mol */
01935         conversion = Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na;
01936
01937         fprintf(file, "elec");
01938         if (Vstring_strcasecmp(nosh->elecname[ielec], "") != 0) {
01939             fprintf(file, " name %s\n", nosh->elecname[ielec]);
01940         } else fprintf(file, "\n");
01941
01942         switch (mgparm->type) {
01943             case MCT_DUMMY:
01944                 fprintf(file, "    mg-dummy\n");
01945                 break;
01946             case MCT_MANUAL:
01947                 fprintf(file, "    mg-manual\n");
01948                 break;
01949             case MCT_AUTO:
01950                 fprintf(file, "    mg-auto\n");
01951                 break;
01952             case MCT_PARALLEL:
01953                 fprintf(file, "    mg-para\n");
01954                 break;
01955             default:
01956                 break;
01957         }
01958
01959         fprintf(file, "    mol %d\n", pbeparm->molid);
01960         fprintf(file, "    dime %d %d %d\n", mgparm->dime[0], mgparm->dime[1],\
01961                 mgparm->dime[2]);
01962
01963         switch (pbeparm->pbetype) {
01964             case PBE_NPBE:
01965                 fprintf(file, "    npbe\n");
01966                 break;
01967             case PBE_LPBE:
01968                 fprintf(file, "    lpbe\n");
01969                 break;
01970             default:
01971                 break;
01972         }
01973
01974         if (pbeparm->nion > 0) {
01975             for (i=0; i<pbeparm->nion; i++) {
01976                 fprintf(file, "    ion %4.3f %4.3f %4.3f\n",
01977                         pbeparm->ionr[i], pbeparm->ionq[i], pbeparm->ionc[i]);
01978             }
01979         }
01980
01981         fprintf(file, "    pdie %4.3f\n", pbeparm->pdie);
01982         fprintf(file, "    sdie %4.3f\n", pbeparm->sdie);
01983
01984         switch (pbeparm->srfm) {
01985             case 0:
01986                 fprintf(file, "    srfm mol\n");
01987                 fprintf(file, "    srad %4.3f\n", pbeparm->srad);
01988                 break;
01989             case 1:
01990                 fprintf(file, "    srfm smol\n");
01991                 fprintf(file, "    srad %4.3f\n", pbeparm->srad);
01992                 break;
01993             case 2:

```

```

01994         fprintf(file, "      srfm spl2\n");
01995         fprintf(file, "      srad %4.3f\n", pbeparm->srad);
01996         break;
01997     default:
01998         break;
01999 }
02000
02001     switch (pbeparm->bcbfl) {
02002     case BCFL_ZERO:
02003         fprintf(file, "      bcbfl zero\n");
02004         break;
02005     case BCFL_SDH:
02006         fprintf(file, "      bcbfl sdh\n");
02007         break;
02008     case BCFL_MDH:
02009         fprintf(file, "      bcbfl mdh\n");
02010         break;
02011     case BCFL_FOCUS:
02012         fprintf(file, "      bcbfl focus\n");
02013         break;
02014     case BCFL_MAP:
02015         fprintf(file, "      bcbfl map\n");
02016         break;
02017     case BCFL_MEM:
02018         fprintf(file, "      bcbfl mem\n");
02019         break;
02020     default:
02021         break;
02022     }
02023
02024     fprintf(file, "      temp %4.3f\n", pbeparm->temp);
02025
02026     for (; icalc<=nosh->elec2calc[ielec]; icalc++){ /* calc loop */
02027
02028         /* Reinitialize per-calc pointers */
02029         mgparm = nosh->calc[icalc]->mgparm;
02030         pbeparm = nosh->calc[icalc]->pbeparm;
02031
02032         fprintf(file, "      calc\n");
02033         fprintf(file, "      id %i\n", (icalc+1));
02034         fprintf(file, "      grid %4.3f %4.3f %4.3f\n",
02035             mgparm->grid[0], mgparm->grid[1], mgparm->grid[2]);
02036         fprintf(file, "      glen %4.3f %4.3f %4.3f\n",
02037             mgparm->glen[0], mgparm->glen[1], mgparm->glen[2]);
02038
02039         if (pbeparm->calcenergy == PCE_TOTAL) {
02040             fprintf(file, "      totEnergy %1.12E kJ/mol\n",
02041                 (totEnergy[icalc]*conversion));
02042         } if (pbeparm->calcenergy == PCE_COMPS) {
02043             fprintf(file, "      totEnergy %1.12E kJ/mol\n",
02044                 (totEnergy[icalc]*conversion));
02045             fprintf(file, "      qfEnergy %1.12E kJ/mol\n",
02046                 (0.5*qfEnergy[icalc]*conversion));
02047             fprintf(file, "      qmEnergy %1.12E kJ/mol\n",
02048                 (qmEnergy[icalc]*conversion));
02049             fprintf(file, "      dielEnergy %1.12E kJ/mol\n",
02050                 (dielEnergy[icalc]*conversion));
02051             for (i=0; i<nenergy[icalc]; i++){
02052                 fprintf(file, "      atom %i %1.12E kJ/mol\n", i,
02053                     (0.5*atomEnergy[icalc][i]*conversion));
02054             }
02055         }
02056     }
02057
02058     if (pbeparm->calcforce == PCF_TOTAL) {
02059         fprintf(file, "      qfForce %1.12E %1.12E %1.12E kJ/mol/A\n",
02060             (atomForce[icalc][0].qfForce[0]*conversion),
02061             (atomForce[icalc][0].qfForce[1]*conversion),
02062             (atomForce[icalc][0].qfForce[2]*conversion));
02063         fprintf(file, "      ibForce %1.12E %1.12E %1.12E kJ/mol/A\n",
02064             (atomForce[icalc][0].ibForce[0]*conversion),
02065             (atomForce[icalc][0].ibForce[1]*conversion),
02066             (atomForce[icalc][0].ibForce[2]*conversion));
02067         fprintf(file, "      dbForce %1.12E %1.12E %1.12E kJ/mol/A\n",
02068             (atomForce[icalc][0].dbForce[0]*conversion),
02069             (atomForce[icalc][0].dbForce[1]*conversion),
02070             (atomForce[icalc][0].dbForce[2]*conversion));
02071     }
02072     fprintf(file, "      end\n");
02073 }
02074

```

```

02075         fprintf(file,"end\n");
02076     }
02077
02078     /* Handle print energy statements */
02079
02080     for (i=0; i<nosh->nprint; i++) {
02081
02082         if (nosh->printwhat[i] == NPT_ENERGY) {
02083
02084             fprintf(file,"print energy");
02085             fprintf(file," %d", nosh->printcalc[i][0]+1);
02086
02087             for (j=1; j<nosh->printnarg[i]; j++) {
02088                 if (nosh->printop[i][j-1] == 0) fprintf(file," +");
02089                 else if (nosh->printop[i][j-1] == 1) fprintf(file," -");
02090                 fprintf(file," %d", nosh->printcalc[i][j]+1);
02091             }
02092
02093             fprintf(file," \n");
02094             icalc = nosh->elec2calc[nosh->printcalc[i][0]];
02095
02096             ltenergy = Vunit_kb * (1e-3) * Vunit_Na * \
02097                 nosh->calc[icalc]->pbeparm->temp * totEnergy[icalc];
02098
02099             for (j=1; j<nosh->printnarg[i]; j++) {
02100                 icalc = nosh->elec2calc[nosh->printcalc[i][j]];
02101                 /* Add or subtract? */
02102                 if (nosh->printop[i][j-1] == 0) scalar = 1.0;
02103                 else if (nosh->printop[i][j-1] == 1) scalar = -1.0;
02104                 /* Accumulate */
02105                 ltenergy += (scalar * Vunit_kb * (1e-3) * Vunit_Na *
02106                     nosh->calc[icalc]->pbeparm->temp * totEnergy[icalc]);
02107
02108                 Vcom_reduce(com, &ltenergy, &gtenergy, 1, 2, 0);
02109             }
02110             fprintf(file,"    localEnergy %1.12E kJ/mol\n", \
02111                 ltenergy);
02112             fprintf(file,"    globalEnergy %1.12E kJ/mol\nend\n", \
02113                 gtenergy);
02114         }
02115     }
02116 }
02117
02118 fclose(file);
02119
02120 return 1;
02121 }
02122
02123 VPUBLIC int writedataXML(Nosh *nosh, Vcom *com, const char *fname,
02124     double totEnergy[NOSH_MAXCALC],
02125     double qfEnergy[NOSH_MAXCALC],
02126     double qmEnergy[NOSH_MAXCALC],
02127     double dielEnergy[NOSH_MAXCALC],
02128     int nenergy[NOSH_MAXCALC],
02129     double *atomEnergy[NOSH_MAXCALC],
02130     int nforce[NOSH_MAXCALC],
02131     AtomForce *atomForce[NOSH_MAXCALC]) {
02132
02133     FILE *file;
02134     time_t now;
02135     int ielec, icalc, i, j;
02136     char *timestring = VNULL;
02137     char *c = VNULL;
02138     PBeparm *pbeparm = VNULL;
02139     MGparm *mgparm = VNULL;
02140     double conversion, ltenergy, gtenergy, scalar;
02141
02142     if (nosh->bogus) return 1;
02143
02144     /* Initialize some variables */
02145
02146     icalc = 0;
02147
02148     file = fopen(fname, "w");
02149     if (file == VNULL) {
02150         Vnm_print(2, "writedataXML: Problem opening virtual socket %s\n",
02151             fname);
02152         return 0;
02153     }
02154
02155     fprintf(file,"<?xml version=\"1.0\" encoding=\"UTF-8\"?>\n");

```



```

02156     fprintf(file, "<APBS>\n");
02157
02158     /* Strip the newline character from the date */
02159
02160     now = time(VNULL);
02161     timestring = ctime(&now);
02162     for(c = timestring; *c != '\n'; c++);
02163     *c = '\0';
02164     fprintf(file, "    <date>%s</date>\n", timestring);
02165
02166     for (ielec=0; ielec<nosh->nelec;ielec++){ /* elec loop */
02167
02168         /* Initialize per-elec pointers */
02169
02170         mgparm = nosh->calc[icalc]->mgparm;
02171         pbeparm = nosh->calc[icalc]->pbeparm;
02172
02173         /* Convert from kT/e to kJ/mol */
02174         conversion = Vunit_kb*pbeparm->temp*(1e-3)*Vunit_Na;
02175
02176         fprintf(file, "    <elec>\n");
02177         if (Vstring_strcasecmp(nosh->elecname[ielec], "") != 0) {
02178             fprintf(file, "    <name>%s</name>\n", nosh->elecname[ielec]);
02179         }
02180
02181         switch (mgparm->type) {
02182             case MCT_DUMMY:
02183                 fprintf(file, "    <type>mg-dummy</type>\n");
02184                 break;
02185             case MCT_MANUAL:
02186                 fprintf(file, "    <type>mg-manual</type>\n");
02187                 break;
02188             case MCT_AUTO:
02189                 fprintf(file, "    <type>mg-auto</type>\n");
02190                 break;
02191             case MCT_PARALLEL:
02192                 fprintf(file, "    <type>mg-para</type>\n");
02193                 break;
02194             default:
02195                 break;
02196         }
02197
02198         fprintf(file, "    <molid>%d</molid>\n", pbeparm->molid);
02199         fprintf(file, "    <nx>%d</nx>\n", mgparm->dime[0]);
02200         fprintf(file, "    <ny>%d</ny>\n", mgparm->dime[1]);
02201         fprintf(file, "    <nz>%d</nz>\n", mgparm->dime[2]);
02202
02203         switch (pbeparm->pbetype) {
02204             case PBE_NPBE:
02205                 fprintf(file, "    <pbe>npbe</pbe>\n");
02206                 break;
02207             case PBE_LPBE:
02208                 fprintf(file, "    <pbe>lpbe</pbe>\n");
02209                 break;
02210             default:
02211                 break;
02212         }
02213
02214         if (pbeparm->nion > 0) {
02215             for (i=0; i<pbeparm->nion; i++) {
02216                 fprintf(file, "    <ion>\n");
02217                 fprintf(file, "    <radius>%4.3f A</radius>\n",
02218                     pbeparm->ionr[i]);
02219                 fprintf(file, "    <charge>%4.3f A</charge>\n",
02220                     pbeparm->ionq[i]);
02221                 fprintf(file, "    <concentration>%4.3f M</concentration>\n",
02222                     pbeparm->ionc[i]);
02223                 fprintf(file, "    </ion>\n");
02224             }
02225         }
02226     }
02227
02228     fprintf(file, "    <pdie>%4.3f</pdie>\n", pbeparm->pdie);
02229     fprintf(file, "    <sdie>%4.3f</sdie>\n", pbeparm->sdie);
02230
02231     switch (pbeparm->srfrm) {
02232         case 0:
02233             fprintf(file, "    <srfrm>mol</srfrm>\n");
02234             fprintf(file, "    <srad>%4.3f</srad>\n", pbeparm->srad);
02235             break;
02236         case 1:

```

```

02237         fprintf(file, "        <srfm>smol</srfm>\n");
02238         fprintf(file, "        <srad>%4.3f</srad>\n", pbeparm->srad);
02239         break;
02240     case 2:
02241         fprintf(file, "        <srfm>spl2</srfm>\n");
02242         break;
02243     default:
02244         break;
02245 }
02246
02247 switch (pbeparm->bcbfl) {
02248     case BCFL_ZERO:
02249         fprintf(file, "        <bcbfl>zero</bcbfl>\n");
02250         break;
02251     case BCFL_SDH:
02252         fprintf(file, "        <bcbfl>sdh</bcbfl>\n");
02253         break;
02254     case BCFL_MDH:
02255         fprintf(file, "        <bcbfl>mdh</bcbfl>\n");
02256         break;
02257     case BCFL_FOCUS:
02258         fprintf(file, "        <bcbfl>focus</bcbfl>\n");
02259         break;
02260     case BCFL_MAP:
02261         fprintf(file, "        <bcbfl>map</bcbfl>\n");
02262         break;
02263     case BCFL_MEM:
02264         fprintf(file, "        <bcbfl>mem</bcbfl>\n");
02265         break;
02266     default:
02267         break;
02268 }
02269
02270 fprintf(file, "        <temp>%4.3f K</temp>\n", pbeparm->temp);
02271
02272 for (; icalc<=nosh->elec2calc[ielec]; icalc++){ /* calc loop */
02273
02274     /* Reinitialize per-calc pointers */
02275     mgparm = nosh->calc[icalc]->mgparm;
02276     pbeparm = nosh->calc[icalc]->pbeparm;
02277
02278     fprintf(file, "        <calc>\n");
02279     fprintf(file, "        <id>%i</id>\n", (icalc+1));
02280     fprintf(file, "        <hx>%4.3f A</hx>\n", mgparm->grid[0]);
02281     fprintf(file, "        <hy>%4.3f A</hy>\n", mgparm->grid[1]);
02282     fprintf(file, "        <hz>%4.3f A</hz>\n", mgparm->grid[2]);
02283     fprintf(file, "        <xlen>%4.3f A</xlen>\n", mgparm->glen[0]);
02284     fprintf(file, "        <ylen>%4.3f A</ylen>\n", mgparm->glen[1]);
02285     fprintf(file, "        <zlen>%4.3f A</zlen>\n", mgparm->glen[2]);
02286
02287     if (pbeparm->calcenergy == PCE_TOTAL) {
02288         fprintf(file, "        <totEnergy>%1.12E kJ/mol</totEnergy>\n",
02289             (totEnergy[icalc]*conversion));
02290     } else if (pbeparm->calcenergy == PCE_COMPS) {
02291         fprintf(file, "        <totEnergy>%1.12E kJ/mol</totEnergy>\n",
02292             (totEnergy[icalc]*conversion));
02293         fprintf(file, "        <qfEnergy>%1.12E kJ/mol</qfEnergy>\n",
02294             (0.5*qfEnergy[icalc]*conversion));
02295         fprintf(file, "        <qmEnergy>%1.12E kJ/mol</qmEnergy>\n",
02296             (qmEnergy[icalc]*conversion));
02297         fprintf(file, "        <dielEnergy>%1.12E kJ/mol</dielEnergy>\n",
02298             (dielEnergy[icalc]*conversion));
02299         for (i=0; i<nenergy[icalc]; i++){
02300             fprintf(file, "        <atom>\n");
02301             fprintf(file, "            <id>%i</id>\n", i+1);
02302             fprintf(file, "            <energy>%1.12E kJ/mol</energy>\n",
02303                 (0.5*atomEnergy[icalc][i]*conversion));
02304             fprintf(file, "        </atom>\n");
02305         }
02306     }
02307
02308
02309     if (pbeparm->calcforce == PCF_TOTAL) {
02310         fprintf(file, "        <qfforce_x>%1.12E</qfforce_x>\n",
02311             atomForce[icalc][0].qfForce[0]*conversion);
02312         fprintf(file, "        <qfforce_y>%1.12E</qfforce_y>\n",
02313             atomForce[icalc][0].qfForce[1]*conversion);
02314         fprintf(file, "        <qfforce_z>%1.12E</qfforce_z>\n",
02315             atomForce[icalc][0].qfForce[2]*conversion);
02316         fprintf(file, "        <ibforce_x>%1.12E</ibforce_x>\n",
02317             atomForce[icalc][0].ibForce[0]*conversion);

```

```

02318             fprintf(file, "                <ibforce_y>%1.12E</ibforce_y>\n",
02319                        atomForce[icalc][0].ibForce[1]*conversion);
02320             fprintf(file, "                <ibforce_z>%1.12E</ibforce_z>\n",
02321                        atomForce[icalc][0].ibForce[2]*conversion);
02322             fprintf(file, "                <dbforce_x>%1.12E</dbforce_x>\n",
02323                        atomForce[icalc][0].dbForce[0]*conversion);
02324             fprintf(file, "                <dbforce_y>%1.12E</dbforce_y>\n",
02325                        atomForce[icalc][0].dbForce[1]*conversion);
02326             fprintf(file, "                <dbforce_z>%1.12E</dbforce_z>\n",
02327                        atomForce[icalc][0].dbForce[2]*conversion);
02328         }
02329
02330         fprintf(file, "            </calc>\n");
02331     }
02332
02333     fprintf(file, "    </elec>\n");
02334 }
02335
02336 /* Handle print energy statements */
02337
02338 for (i=0; i<nosh->nprint; i++) {
02339
02340     if (nosh->printwhat[i] == NPT_ENERGY) {
02341
02342         fprintf(file, "        <printEnergy>\n");
02343         fprintf(file, "        <equation>%d", nosh->printcalc[i][0]+1);
02344
02345         for (j=1; j<nosh->printnarg[i]; j++) {
02346             if (nosh->printop[i][j-1] == 0) fprintf(file, " +");
02347             else if (nosh->printop[i][j-1] == 1) fprintf(file, " -");
02348             fprintf(file, " %d", nosh->printcalc[i][j] +1);
02349         }
02350
02351         fprintf(file, "</equation>\n");
02352         icalc = nosh->elec2calc[nosh->printcalc[i][0]];
02353
02354         ltenergy = Vunit_kb * (1e-3) * Vunit_Na * \
02355             nosh->calc[icalc]->pbeparm->temp * totEnergy[icalc];
02356
02357         for (j=1; j<nosh->printnarg[i]; j++) {
02358             icalc = nosh->elec2calc[nosh->printcalc[i][j]];
02359             /* Add or subtract? */
02360             if (nosh->printop[i][j-1] == 0) scalar = 1.0;
02361             else if (nosh->printop[i][j-1] == 1) scalar = -1.0;
02362             /* Accumulate */
02363             ltenergy += (scalar * Vunit_kb * (1e-3) * Vunit_Na *
02364                         nosh->calc[icalc]->pbeparm->temp * totEnergy[icalc]);
02365         }
02366         Vcom_reduce(com, &ltenergy, &gtenergy, 1, 2, 0);
02367         fprintf(file, "        <localEnergy>%1.12E kJ/mol</localEnergy>\n", \
02368                 ltenergy);
02369         fprintf(file, "        <globalEnergy>%1.12E kJ/mol</globalEnergy>\n", \
02370                 gtenergy);
02371
02372         fprintf(file, "    </printEnergy>\n");
02373     }
02374 }
02375
02376 /* Add ending tags and close the file */
02377 fprintf(file, "</APBS>\n");
02378 fclose(file);
02379
02380 return 1;
02381 }
02382
02383 VPUBLIC int writedataMG(int rank,
02384                        Nosh *nosh,
02385                        PBEParm *pbeparm,
02386                        Vpmg *pmg
02387                        ) {
02388
02389     char writestem[VMAX_ARGLEN];
02390     char outpath[VMAX_ARGLEN];
02391     char title[72];
02392     int i,
02393         nx,
02394         ny,
02395         nz,
02396         natoms;
02397     double hx,
02398         hy,

```

```

02399         hzed,
02400         xcent,
02401         ycent,
02402         zcent,
02403         xmin,
02404         ymin,
02405         zmin;
02406
02407     Vgrid *grid;
02408     Vio *sock;
02409
02410     if (nosh->bogus) return 1;
02411
02412     for (i=0; i<pbeparm->numwrite; i++) {
02413
02414         nx = pmg->pmgp->nx;
02415         ny = pmg->pmgp->ny;
02416         nz = pmg->pmgp->nz;
02417         hx = pmg->pmgp->hx;
02418         hy = pmg->pmgp->hy;
02419         hzed = pmg->pmgp->hzed;
02420
02421         switch (pbeparm->writetype[i]) {
02422
02423             case VDT_CHARGE:
02424
02425                 Vnm_tprint(1, " Writing charge distribution to ");
02426                 xcent = pmg->pmgp->xcent;
02427                 ycent = pmg->pmgp->ycent;
02428                 zcent = pmg->pmgp->zcent;
02429                 xmin = xcent - 0.5*(nx-1)*hx;
02430                 ymin = ycent - 0.5*(ny-1)*hy;
02431                 zmin = zcent - 0.5*(nz-1)*hzed;
02432                 VASSERT(Vpmg_fillArray(pmg, pmg->rwork, VDT_CHARGE, 0.0,
02433                                     pbeparm->pbetype, pbeparm));
02434                 sprintf(title, "CHARGE DISTRIBUTION (e)");
02435                 break;
02436
02437             case VDT_POT:
02438
02439                 Vnm_tprint(1, " Writing potential to ");
02440                 xcent = pmg->pmgp->xcent;
02441                 ycent = pmg->pmgp->ycent;
02442                 zcent = pmg->pmgp->zcent;
02443                 xmin = xcent - 0.5*(nx-1)*hx;
02444                 ymin = ycent - 0.5*(ny-1)*hy;
02445                 zmin = zcent - 0.5*(nz-1)*hzed;
02446                 VASSERT(Vpmg_fillArray(pmg, pmg->rwork, VDT_POT, 0.0,
02447                                     pbeparm->pbetype, pbeparm));
02448                 sprintf(title, "POTENTIAL (kT/e)");
02449                 break;
02450
02451             case VDT_SMOL:
02452
02453                 Vnm_tprint(1, " Writing molecular accessibility to ");
02454                 xcent = pmg->pmgp->xcent;
02455                 ycent = pmg->pmgp->ycent;
02456                 zcent = pmg->pmgp->zcent;
02457                 xmin = xcent - 0.5*(nx-1)*hx;
02458                 ymin = ycent - 0.5*(ny-1)*hy;
02459                 zmin = zcent - 0.5*(nz-1)*hzed;
02460                 VASSERT(Vpmg_fillArray(pmg, pmg->rwork, VDT_SMOL,
02461                                     pbeparm->srad, pbeparm->pbetype, pbeparm));
02462                 sprintf(title,
02463                         "SOLVENT ACCESSIBILITY -- MOLECULAR (%4.3f PROBE)",
02464                         pbeparm->srad);
02465                 break;
02466
02467             case VDT_SSPL:
02468
02469                 Vnm_tprint(1, " Writing spline-based accessibility to ");
02470                 xcent = pmg->pmgp->xcent;
02471                 ycent = pmg->pmgp->ycent;
02472                 zcent = pmg->pmgp->zcent;
02473                 xmin = xcent - 0.5*(nx-1)*hx;
02474                 ymin = ycent - 0.5*(ny-1)*hy;
02475                 zmin = zcent - 0.5*(nz-1)*hzed;
02476                 VASSERT(Vpmg_fillArray(pmg, pmg->rwork, VDT_SSPL,
02477                                     pbeparm->swin, pbeparm->pbetype, pbeparm));
02478                 sprintf(title,
02479                         "SOLVENT ACCESSIBILITY -- SPLINE (%4.3f WINDOW)",

```

```
02480         pbeparm->swin);
02481     break;
02482
02483     case VDT_VDW:
02484
02485         Vnm_tprint(1, " Writing van der Waals accessibility to ");
02486         xcent = pmg->pmgp->xcent;
02487         ycent = pmg->pmgp->ycent;
02488         zcent = pmg->pmgp->zcent;
02489         xmin = xcent - 0.5*(nx-1)*hx;
02490         ymin = ycent - 0.5*(ny-1)*hy;
02491         zmin = zcent - 0.5*(nz-1)*hz;
02492         VASSERT(Vpmg_fillArray(pmg, pmg->rwork, VDT_VDW, 0.0,
02493                               pbeparm->pbetype, pbeparm));
02494         sprintf(title, "SOLVENT ACCESSIBILITY -- VAN DER WAALS");
02495         break;
02496
02497     case VDT_IVDW:
02498
02499         Vnm_tprint(1, " Writing ion accessibility to ");
02500         xcent = pmg->pmgp->xcent;
02501         ycent = pmg->pmgp->ycent;
02502         zcent = pmg->pmgp->zcent;
02503         xmin = xcent - 0.5*(nx-1)*hx;
02504         ymin = ycent - 0.5*(ny-1)*hy;
02505         zmin = zcent - 0.5*(nz-1)*hz;
02506         VASSERT(Vpmg_fillArray(pmg, pmg->rwork, VDT_IVDW,
02507                               pmg->pbe->maxIonRadius, pbeparm->pbetype, pbeparm));
02508         sprintf(title,
02509                 "ION ACCESSIBILITY -- SPLINE (%4.3f RADIUS)",
02510                 pmg->pbe->maxIonRadius);
02511         break;
02512
02513     case VDT_LAP:
02514
02515         Vnm_tprint(1, " Writing potential Laplacian to ");
02516         xcent = pmg->pmgp->xcent;
02517         ycent = pmg->pmgp->ycent;
02518         zcent = pmg->pmgp->zcent;
02519         xmin = xcent - 0.5*(nx-1)*hx;
02520         ymin = ycent - 0.5*(ny-1)*hy;
02521         zmin = zcent - 0.5*(nz-1)*hz;
02522         VASSERT(Vpmg_fillArray(pmg, pmg->rwork, VDT_LAP, 0.0,
02523                               pbeparm->pbetype, pbeparm));
02524         sprintf(title,
02525                 "POTENTIAL LAPLACIAN (kT/e/A^2)");
02526         break;
02527
02528     case VDT_EDENS:
02529
02530         Vnm_tprint(1, " Writing energy density to ");
02531         xcent = pmg->pmgp->xcent;
02532         ycent = pmg->pmgp->ycent;
02533         zcent = pmg->pmgp->zcent;
02534         xmin = xcent - 0.5*(nx-1)*hx;
02535         ymin = ycent - 0.5*(ny-1)*hy;
02536         zmin = zcent - 0.5*(nz-1)*hz;
02537         VASSERT(Vpmg_fillArray(pmg, pmg->rwork, VDT_EDENS, 0.0,
02538                               pbeparm->pbetype, pbeparm));
02539         sprintf(title, "ENERGY DENSITY (kT/e/A)^2");
02540         break;
02541
02542     case VDT_NDENS:
02543
02544         Vnm_tprint(1, " Writing number density to ");
02545         xcent = pmg->pmgp->xcent;
02546         ycent = pmg->pmgp->ycent;
02547         zcent = pmg->pmgp->zcent;
02548         xmin = xcent - 0.5*(nx-1)*hx;
02549         ymin = ycent - 0.5*(ny-1)*hy;
02550         zmin = zcent - 0.5*(nz-1)*hz;
02551         VASSERT(Vpmg_fillArray(pmg, pmg->rwork, VDT_NDENS, 0.0,
02552                               pbeparm->pbetype, pbeparm));
02553         sprintf(title,
02554                 "ION NUMBER DENSITY (M)");
02555         break;
02556
02557     case VDT_QDENS:
02558
02559         Vnm_tprint(1, " Writing charge density to ");
02560         xcent = pmg->pmgp->xcent;
```

```

02561         ycent = pmg->pmgp->ycent;
02562         zcent = pmg->pmgp->zcent;
02563         xmin = xcent - 0.5*(nx-1)*hx;
02564         ymin = ycent - 0.5*(ny-1)*hy;
02565         zmin = zcent - 0.5*(nz-1)*hzed;
02566         VASSERT(Vpmg_fillArray(pmg, pmg->rwork, VDT_QDENS, 0.0,
02567                               pbeparm->pbetype, pbeparm));
02568         sprintf(title,
02569                 "ION CHARGE DENSITY (e_c * M)");
02570         break;
02571
02572     case VDT_DIELX:
02573
02574         Vnm_tprint(1, " Writing x-shifted dielectric map to ");
02575         xcent = pmg->pmgp->xcent + 0.5*hx;
02576         ycent = pmg->pmgp->ycent;
02577         zcent = pmg->pmgp->zcent;
02578         xmin = xcent - 0.5*(nx-1)*hx;
02579         ymin = ycent - 0.5*(ny-1)*hy;
02580         zmin = zcent - 0.5*(nz-1)*hzed;
02581         VASSERT(Vpmg_fillArray(pmg, pmg->rwork, VDT_DIELX, 0.0,
02582                               pbeparm->pbetype, pbeparm));
02583         sprintf(title,
02584                 "X-SHIFTED DIELECTRIC MAP");
02585         break;
02586
02587     case VDT_DIELY:
02588
02589         Vnm_tprint(1, " Writing y-shifted dielectric map to ");
02590         xcent = pmg->pmgp->xcent;
02591         ycent = pmg->pmgp->ycent + 0.5*hy;
02592         zcent = pmg->pmgp->zcent;
02593         xmin = xcent - 0.5*(nx-1)*hx;
02594         ymin = ycent - 0.5*(ny-1)*hy;
02595         zmin = zcent - 0.5*(nz-1)*hzed;
02596         VASSERT(Vpmg_fillArray(pmg, pmg->rwork, VDT_DIELY, 0.0,
02597                               pbeparm->pbetype, pbeparm));
02598         sprintf(title,
02599                 "Y-SHIFTED DIELECTRIC MAP");
02600         break;
02601
02602     case VDT_DIELZ:
02603
02604         Vnm_tprint(1, " Writing z-shifted dielectric map to ");
02605         xcent = pmg->pmgp->xcent;
02606         ycent = pmg->pmgp->ycent;
02607         zcent = pmg->pmgp->zcent + 0.5*hzed;
02608         xmin = xcent - 0.5*(nx-1)*hx;
02609         ymin = ycent - 0.5*(ny-1)*hy;
02610         zmin = zcent - 0.5*(nz-1)*hzed;
02611         VASSERT(Vpmg_fillArray(pmg, pmg->rwork, VDT_DIELZ, 0.0,
02612                               pbeparm->pbetype, pbeparm));
02613         sprintf(title,
02614                 "Z-SHIFTED DIELECTRIC MAP");
02615         break;
02616
02617     case VDT_KAPPA:
02618
02619         Vnm_tprint(1, " Writing kappa map to ");
02620         xcent = pmg->pmgp->xcent;
02621         ycent = pmg->pmgp->ycent;
02622         zcent = pmg->pmgp->zcent;
02623         xmin = xcent - 0.5*(nx-1)*hx;
02624         ymin = ycent - 0.5*(ny-1)*hy;
02625         zmin = zcent - 0.5*(nz-1)*hzed;
02626         VASSERT(Vpmg_fillArray(pmg, pmg->rwork, VDT_KAPPA, 0.0,
02627                               pbeparm->pbetype, pbeparm));
02628         sprintf(title,
02629                 "KAPPA MAP");
02630         break;
02631
02632     case VDT_ATOMPOT:
02633
02634         Vnm_tprint(1, " Writing atom potentials to ");
02635         xcent = pmg->pmgp->xcent;
02636         ycent = pmg->pmgp->ycent;
02637         zcent = pmg->pmgp->zcent;
02638         xmin = xcent - 0.5*(nx-1)*hx;
02639         ymin = ycent - 0.5*(ny-1)*hy;
02640         zmin = zcent - 0.5*(nz-1)*hzed;
02641         VASSERT(Vpmg_fillArray(pmg, pmg->rwork, VDT_ATOMPOT, 0.0,

```

```

02642                                     pbeparm->pbetype, pbeparm));
02643         sprintf(title,
02644                 "ATOM POTENTIALS");
02645         break;
02646     default:
02647
02648         Vnm_tprint(2, "Invalid data type for writing!\n");
02649         return 0;
02650     }
02651
02652
02653 #ifdef HAVE_MPI_H
02654     sprintf(writestem, "%s-PE%d", pbeparm->writestem[i], rank);
02655 #else
02656     if(nosh->ispara){
02657         sprintf(writestem, "%s-PE%d", pbeparm->writestem[i], nosh->proc_rank);
02658     }else{
02659         sprintf(writestem, "%s", pbeparm->writestem[i]);
02660     }
02661 #endif
02662
02663     switch (pbeparm->writefmt[i]) {
02664
02665     case VDF_DX:
02666         sprintf(outpath, "%s.%s", writestem, "dx");
02667         Vnm_tprint(1, "%s\n", outpath);
02668         grid = Vgrid_ctor(nx, ny, nz, hx, hy, hzed, xmin, ymin, zmin,
02669                          pmg->rwork);
02670         Vgrid_writeDX(grid, "FILE", "ASC", VNULL, outpath, title,
02671                      pmg->pvec);
02672         Vgrid_dtor(&grid);
02673         break;
02674
02675     case VDF_DXBIN:
02676         sprintf(outpath, "%s.%s", writestem, "dxbin");
02677         Vnm_tprint(1, "%s\n", outpath);
02678         grid = Vgrid_ctor(nx, ny, nz, hx, hy, hzed, xmin, ymin, zmin,
02679                          pmg->rwork);
02680         //TODO: write Vgrid_writeDXBIN method
02681         Vgrid_writeDXBIN(grid, "FILE", "ASC", VNULL, outpath, title,
02682                          pmg->pvec);
02683         Vgrid_dtor(&grid);
02684         break;
02685
02686     case VDF_AVS:
02687         sprintf(outpath, "%s.%s", writestem, "ucd");
02688         Vnm_tprint(1, "%s\n", outpath);
02689         Vnm_tprint(2, "Sorry, AVS format isn't supported for \
02690 uniform meshes yet!\n");
02691         break;
02692
02693     case VDF_MCSF:
02694         sprintf(outpath, "%s.%s", writestem, "mcsf");
02695         Vnm_tprint(1, "%s\n", outpath);
02696         Vnm_tprint(2, "Sorry, MCSF format isn't supported for \
02697 uniform meshes yet!\n");
02698         break;
02699
02700     case VDF_UHBD:
02701         sprintf(outpath, "%s.%s", writestem, "grd");
02702         Vnm_tprint(1, "%s\n", outpath);
02703         grid = Vgrid_ctor(nx, ny, nz, hx, hy, hzed, xmin, ymin, zmin,
02704                          pmg->rwork);
02705         Vgrid_writeUHBD(grid, "FILE", "ASC", VNULL, outpath, title,
02706                          pmg->pvec);
02707         Vgrid_dtor(&grid);
02708         break;
02709
02710     case VDF_GZ:
02711         sprintf(outpath, "%s.%s", writestem, "dx.gz");
02712         Vnm_tprint(1, "%s\n", outpath);
02713         grid = Vgrid_ctor(nx, ny, nz, hx, hy, hzed, xmin, ymin, zmin,
02714                          pmg->rwork);
02715         Vgrid_writeGZ(grid, "FILE", "ASC", VNULL, outpath, title,
02716                       pmg->pvec);
02717         Vgrid_dtor(&grid);
02718         break;
02719     case VDF_FLAT:
02720         sprintf(outpath, "%s.%s", writestem, "txt");
02721         Vnm_tprint(1, "%s\n", outpath);
02722         Vnm_print(0, "routines: Opening virtual socket...\n");

```

```

02723         sock = Vio_ctor("FILE", "ASC", VNULL, outpath, "w");
02724         if (sock == VNULL) {
02725             Vnm_print(2, "routines: Problem opening virtual socket %s\n",
02726                 outpath);
02727             return 0;
02728         }
02729         if (Vio_connect(sock, 0) < 0) {
02730             Vnm_print(2, "routines: Problem connecting virtual socket %s\n",
02731                 outpath);
02732             return 0;
02733         }
02734         Vio_printf(sock, "# Data from %s\n", PACKAGE_STRING);
02735         Vio_printf(sock, "# \n");
02736         Vio_printf(sock, "# %s\n", title);
02737         Vio_printf(sock, "# \n");
02738         natoms = pmg->pbe->alist[pbeparm->molid-1].number;
02739         for (i=0; i<natoms; i++)
02740             Vio_printf(sock, "%12.6e\n", pmg->rwork[i]);
02741         break;
02742     default:
02743         Vnm_tprint(2, "Bogus data format (%d)!\n",
02744             pbeparm->writefmt[i]);
02745         break;
02746     }
02747 }
02748 }
02749
02750 return 1;
02751 }
02752
02753 VPUBLIC double returnEnergy(Vcom *com,
02754     Nosh *nosh,
02755     double totEnergy[NOSH_MAXCALC],
02756     int iprint
02757 ) {
02758
02759     int iarg,
02760         calcid;
02761     double ltenergy,
02762         scalar;
02763
02764     calcid = nosh->elec2calc[nosh->printcalc[iprint][0]];
02765     if (nosh->calc[calcid]->pbeparm->calcenergy != PCE_NO) {
02766         ltenergy = Vunit_kb * (1e-3) * Vunit_Na *
02767             nosh->calc[calcid]->pbeparm->temp * totEnergy[calcid];
02768     } else {
02769         Vnm_tprint( 2, " No energy available in Calculation %d\n", calcid+1);
02770         return 0.0;
02771     }
02772     for (iarg=1; iarg<nosh->printnarg[iprint]; iarg++){
02773         calcid = nosh->elec2calc[nosh->printcalc[iprint][iarg]];
02774         /* Add or subtract */
02775         if (nosh->printtop[iprint][iarg-1] == 0) scalar = 1.0;
02776         else if (nosh->printtop[iprint][iarg-1] == 1) scalar = -1.0;
02777         /* Accumulate */
02778         ltenergy += (scalar * Vunit_kb * (1e-3) * Vunit_Na *
02779             nosh->calc[calcid]->pbeparm->temp * totEnergy[calcid]);
02780     }
02781
02782     return ltenergy;
02783 }
02784
02785 VPUBLIC int printEnergy(Vcom *com,
02786     Nosh *nosh,
02787     double totEnergy[NOSH_MAXCALC],
02788     int iprint
02789 ) {
02790
02791     int iarg,
02792         calcid;
02793     double ltenergy,
02794         gtenergy,
02795         scalar;
02796
02797     Vnm_tprint( 2, "Warning: The 'energy' print keyword is deprecated.\n" \
02798         "           Use eilecEnergy for electrostatics energy calcs.\n\n");
02799
02800     if (Vstring_strcasecmp(nosh->elecname[nosh->printcalc[iprint][0]], "") == 0) {
02801         Vnm_tprint( 1, "print energy %d ", nosh->printcalc[iprint][0]+1);
02802     } else {
02803         Vnm_tprint( 1, "print energy %d (%s) ", nosh->printcalc[iprint][0]+1,

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```

02804         nosh->elecname[nosh->printcalc[iprint][0]]);
02805     }
02806     for (iarg=1; iarg<nosh->printnarg[iprint]; iarg++) {
02807         if (nosh->printop[iprint][iarg-1] == 0)
02808             Vnm_tprint(1, "+ ");
02809         else if (nosh->printop[iprint][iarg-1] == 1)
02810             Vnm_tprint(1, "- ");
02811         else {
02812             Vnm_tprint( 2, "Undefined PRINT operation!\n");
02813             return 0;
02814         }
02815         if (Vstring_strcasecmp(nosh->elecname[nosh->printcalc[iprint][iarg]],
02816                               "") == 0) {
02817             Vnm_tprint( 1, "%d ", nosh->printcalc[iprint][iarg]+1);
02818         } else {
02819             Vnm_tprint( 1, "%d (%s) ", nosh->printcalc[iprint][iarg]+1,
02820                       nosh->elecname[nosh->printcalc[iprint][iarg]]);
02821         }
02822     }
02823     Vnm_tprint(1, "end\n");
02824     calcid = nosh->elec2calc[nosh->printcalc[iprint][0]];
02825     if (nosh->calc[calcid]->pbeparm->calcenergy != PCE_NO) {
02826         ltenergy = Vunit_kb * (1e-3) * Vunit_Na *
02827             nosh->calc[calcid]->pbeparm->temp * totEnergy[calcid];
02828     } else {
02829         Vnm_tprint( 2, " Didn't calculate energy in Calculation \
02830 #d\n", calcid+1);
02831         return 0;
02832     }
02833     for (iarg=1; iarg<nosh->printnarg[iprint]; iarg++) {
02834         calcid = nosh->elec2calc[nosh->printcalc[iprint][iarg]];
02835         /* Add or subtract? */
02836         if (nosh->printop[iprint][iarg-1] == 0) scalar = 1.0;
02837         else if (nosh->printop[iprint][iarg-1] == 1) scalar = -1.0;
02838         /* Accumulate */
02839         ltenergy += (scalar * Vunit_kb * (1e-3) * Vunit_Na *
02840                     nosh->calc[calcid]->pbeparm->temp * totEnergy[calcid]);
02841     }
02842     Vnm_tprint( 1, " Local net energy (PE %d) = %1.12E kJ/mol\n",
02843               Vcom_rank(com), ltenergy);
02844     Vnm_tprint( 0, "printEnergy: Performing global reduction (sum)\n");
02845     Vcom_reduce(com, &ltenergy, &gtenergy, 1, 2, 0);
02846     Vnm_tprint( 1, " Global net ELEC energy = %1.12E kJ/mol\n", gtenergy);
02847
02848
02849     return 1;
02850 }
02851 }
02852
02853 VPUBLIC int printElecEnergy(Vcom *com,
02854                             Nosh *nosh,
02855                             double totEnergy[NOSH_MAXCALC],
02856                             int iprint
02857                             ) {
02858
02859     int iarg,
02860         calcid;
02861     double ltenergy,
02862         gtenergy,
02863         scalar;
02864
02865     if (Vstring_strcasecmp(nosh->elecname[nosh->printcalc[iprint][0]], "") == 0){
02866         Vnm_tprint( 1, "\nprint energy %d ", nosh->printcalc[iprint][0]+1);
02867     } else {
02868         Vnm_tprint( 1, "\nprint energy %d (%s) ", nosh->printcalc[iprint][0]+1,
02869                   nosh->elecname[nosh->printcalc[iprint][0]]);
02870     }
02871     for (iarg=1; iarg<nosh->printnarg[iprint]; iarg++) {
02872         if (nosh->printop[iprint][iarg-1] == 0)
02873             Vnm_tprint(1, "+ ");
02874         else if (nosh->printop[iprint][iarg-1] == 1)
02875             Vnm_tprint(1, "- ");
02876         else {
02877             Vnm_tprint( 2, "Undefined PRINT operation!\n");
02878             return 0;
02879         }
02880         if (Vstring_strcasecmp(nosh->elecname[nosh->printcalc[iprint][iarg]],
02881                               "") == 0) {
02882             Vnm_tprint( 1, "%d ", nosh->printcalc[iprint][iarg]+1);
02883         } else {
02884             Vnm_tprint( 1, "%d (%s) ", nosh->printcalc[iprint][iarg]+1,

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02885         nosh->elecname[nosh->printcalc[iprint][iarg]]);
02886     }
02887 }
02888 Vnm_tprint(1, "end\n");
02889 calcid = nosh->elec2calc[nosh->printcalc[iprint][0]];
02890 if (nosh->calc[calcid]->pbeparm->calcenergy != PCE_NO) {
02891     ltenergy = Vunit_kb * (1e-3) * Vunit_Na *
02892     nosh->calc[calcid]->pbeparm->temp * totEnergy[calcid];
02893 } else {
02894     Vnm_tprint( 2, " Didn't calculate energy in Calculation \
02895 #d\n", calcid+1);
02896     return 0;
02897 }
02898 for (iarg=1; iarg<nosh->printnarg[iprint]; iarg++) {
02899     calcid = nosh->elec2calc[nosh->printcalc[iprint][iarg]];
02900     /* Add or subtract? */
02901     if (nosh->printop[iprint][iarg-1] == 0) scalar = 1.0;
02902     else if (nosh->printop[iprint][iarg-1] == 1) scalar = -1.0;
02903     /* Accumulate */
02904     ltenergy += (scalar * Vunit_kb * (1e-3) * Vunit_Na *
02905     nosh->calc[calcid]->pbeparm->temp * totEnergy[calcid]);
02906 }
02907 Vnm_tprint( 1, " Local net energy (PE %d) = %1.12E kJ/mol\n",
02908 Vcom_rank(com), ltenergy);
02909 Vnm_tprint( 0, "printEnergy: Performing global reduction (sum)\n");
02910 Vcom_reduce(com, &ltenergy, &gtenergy, 1, 2, 0);
02911 Vnm_tprint( 1, " Global net ELEC energy = %1.12E kJ/mol\n", gtenery);
02912
02913 return 1;
02914 }
02915
02916 }
02917
02918 VPUBLIC int printApolEnergy(Nosh *nosh,
02919 int iprint
02920 ) {
02921
02922     int iarg,
02923     calcid;
02924     double gtenergy,
02925     scalar;
02926     APOLparm *apolparm = VNULL;
02927
02928     if (Vstring_strcasecmp(nosh->apolname[nosh->printcalc[iprint][0]], "") == 0){
02929         Vnm_tprint( 1, "\nprint APOL energy %d ", nosh->printcalc[iprint][0]+1);
02930     } else {
02931         Vnm_tprint( 1, "\nprint APOL energy %d (%s) ", nosh->printcalc[iprint][0]+1,
02932         nosh->apolname[nosh->printcalc[iprint][0]]);
02933     }
02934     for (iarg=1; iarg<nosh->printnarg[iprint]; iarg++) {
02935         if (nosh->printop[iprint][iarg-1] == 0)
02936             Vnm_tprint(1, "+ ");
02937         else if (nosh->printop[iprint][iarg-1] == 1)
02938             Vnm_tprint(1, "- ");
02939         else {
02940             Vnm_tprint( 2, "Undefined PRINT operation!\n");
02941             return 0;
02942         }
02943         if (Vstring_strcasecmp(nosh->apolname[nosh->printcalc[iprint][iarg]],
02944         "") == 0) {
02945             Vnm_tprint( 1, "%d ", nosh->printcalc[iprint][iarg]+1);
02946         } else {
02947             Vnm_tprint( 1, "%d (%s) ", nosh->printcalc[iprint][iarg]+1,
02948             nosh->apolname[nosh->printcalc[iprint][iarg]]);
02949         }
02950     }
02951     Vnm_tprint(1, "end\n");
02952
02953     calcid = nosh->apol2calc[nosh->printcalc[iprint][0]];
02954     apolparm = nosh->calc[calcid]->apolparm;
02955
02956     if (apolparm->calcenergy == ACE_TOTAL) {
02957         gtenergy = ((apolparm->gamma*apolparm->sasa) + (apolparm->press*apolparm->sav) +
02958         (apolparm->wcaEnergy));
02959     } else {
02960         Vnm_tprint( 2, " Didn't calculate energy in Calculation #d\n", calcid+1);
02961         return 0;
02962     }
02963     for (iarg=1; iarg<nosh->printnarg[iprint]; iarg++) {
02964         calcid = nosh->apol2calc[nosh->printcalc[iprint][iarg]];
02965         apolparm = nosh->calc[calcid]->apolparm;

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02965
02966     /* Add or subtract? */
02967     if (nosh->printop[iprint][iarg-1] == 0) scalar = 1.0;
02968     else if (nosh->printop[iprint][iarg-1] == 1) scalar = -1.0;
02969     /* Accumulate */
02970     gtenergy += (scalar * ((apolparm->gamma*apolparm->sasa) +
02971                          (apolparm->press*apolparm->sav) +
02972                          (apolparm->wcaEnergy)));
02973
02974 }
02975
02976 Vnm_tprint( 1, " Global net APOL energy = %1.12E kJ/mol\n", gtenergy);
02977 return 1;
02978 }
02979
02980 VPUBLIC int printForce(Vcom *com,
02981                      NOsh *nosh,
02982                      int nforce[NOSH_MAXCALC],
02983                      AtomForce *atomForce[NOSH_MAXCALC],
02984                      int iprint
02985                      ) {
02986
02987     int iarg,
02988         ifr,
02989         ivc,
02990         calcid,
02991         refnforce,
02992         refcalcf force;
02993     double temp,
02994         scalar,
02995         totforce[3];
02996     AtomForce *lforce,
02997         *gforce,
02998         *aforce;
02999
03000     Vnm_tprint( 2, "Warning: The 'force' print keyword is deprecated.\n" \
03001               " Use elecForce for electrostatics force calcs.\n\n");
03002
03003     if (Vstring_strcasecmp(nosh->elecname[nosh->printcalc[iprint][0]], "") == 0){
03004         Vnm_tprint( 1, "print force %d ", nosh->printcalc[iprint][0]+1);
03005     } else {
03006         Vnm_tprint( 1, "print force %d (%s) ", nosh->printcalc[iprint][0]+1,
03007                   nosh->elecname[nosh->printcalc[iprint][0]]);
03008     }
03009     for (iarg=1; iarg<nosh->printnarg[iprint]; iarg++) {
03010         if (nosh->printop[iprint][iarg-1] == 0)
03011             Vnm_tprint(1, "+ ");
03012         else if (nosh->printop[iprint][iarg-1] == 1)
03013             Vnm_tprint(1, "- ");
03014         else {
03015             Vnm_tprint( 2, "Undefined PRINT operation!\n");
03016             return 0;
03017         }
03018         if (Vstring_strcasecmp(nosh->elecname[nosh->printcalc[iprint][iarg]],
03019                               "") == 0) {
03020             Vnm_tprint( 1, "%d ", nosh->printcalc[iprint][iarg]+1);
03021         } else {
03022             Vnm_tprint( 1, "%d (%s) ", nosh->printcalc[iprint][iarg]+1,
03023                       nosh->elecname[nosh->printcalc[iprint][iarg]]);
03024         }
03025     }
03026     Vnm_tprint(1, "end\n");
03027
03028     /* First, go through and make sure we did the same type of force
03029      * evaluation in each of the requested calculations */
03030     calcid = nosh->elec2calc[nosh->printcalc[iprint][0]];
03031     refnforce = nforce[calcid];
03032     refcalcf force = nosh->calc[calcid]->pbeparm->calcforce;
03033     if (refcalcf force == PCF_NO) {
03034         Vnm_tprint( 2, " Didn't calculate force in calculation \
03035 #d\n", calcid+1);
03036         return 0;
03037     }
03038     for (iarg=1; iarg<nosh->printnarg[iprint]; iarg++) {
03039         calcid = nosh->elec2calc[nosh->printcalc[iprint][iarg]-1];
03040         if (nosh->calc[calcid]->pbeparm->calcforce != refcalcf force) {
03041             Vnm_tprint(2, " Inconsistent calcforce declarations in \
03042 calculations %d and %d\n", nosh->elec2calc[nosh->printcalc[iprint][0]]+1,
03043                       calcid+1);
03044             return 0;
03045         }

```

```

03046         if (nforce[calcid] != refnforce) {
03047             Vnm_tprint(2, " Inconsistent number of forces evaluated in \
03048 calculations %d and %d\n", nosh->elec2calc[nosh->printcalc[iprint][0]]+1,
03049                 calcid+1);
03050             return 0;
03051         }
03052     }
03053
03054     /* Now, allocate space to accumulate the forces */
03055     lforce = (AtomForce *)Vmem_malloc(VNULL, refnforce, sizeof(AtomForce));
03056     gforce = (AtomForce *)Vmem_malloc(VNULL, refnforce, sizeof(AtomForce));
03057
03058     /* Now, accumulate the forces */
03059     calcid = nosh->elec2calc[nosh->printcalc[iprint][0]];
03060     aforce = atomForce[calcid];
03061     temp = nosh->calc[calcid]->pbeparm->temp;
03062
03063     /* Load up the first calculation */
03064     if (refcalcforce == PCF_TOTAL) {
03065         /* Set to total force */
03066         for (ivc=0; ivc<3; ivc++) {
03067             lforce[0].qfForce[ivc] =
03068                 Vunit_kb*(1e-3)*Vunit_Na*temp*aforce[0].qfForce[ivc];
03069             lforce[0].ibForce[ivc] =
03070                 Vunit_kb*(1e-3)*Vunit_Na*temp*aforce[0].ibForce[ivc];
03071             lforce[0].dbForce[ivc] =
03072                 Vunit_kb*(1e-3)*Vunit_Na*temp*aforce[0].dbForce[ivc];
03073         }
03074     } else if (refcalcforce == PCF_COMPS) {
03075         for (ifr=0; ifr<refnforce; ifr++) {
03076             for (ivc=0; ivc<3; ivc++) {
03077                 lforce[ifr].qfForce[ivc] =
03078                     Vunit_kb*(1e-3)*Vunit_Na*temp*aforce[ifr].qfForce[ivc];
03079                 lforce[ifr].ibForce[ivc] =
03080                     Vunit_kb*(1e-3)*Vunit_Na*temp*aforce[ifr].ibForce[ivc];
03081                 lforce[ifr].dbForce[ivc] =
03082                     Vunit_kb*(1e-3)*Vunit_Na*temp*aforce[ifr].dbForce[ivc];
03083             }
03084         }
03085     }
03086
03087     /* Load up the rest of the calculations */
03088     for (iarg=1; iarg<nosh->printnarg[iprint]; iarg++) {
03089         calcid = nosh->elec2calc[nosh->printcalc[iprint][iarg]];
03090         temp = nosh->calc[calcid]->pbeparm->temp;
03091         aforce = atomForce[calcid];
03092         /* Get operation */
03093         if (nosh->printop[iprint][iarg-1] == 0) scalar = +1.0;
03094         else if (nosh->printop[iprint][iarg-1] == 1) scalar = -1.0;
03095         else scalar = 0.0;
03096         /* Accumulate */
03097         if (refcalcforce == PCF_TOTAL) {
03098             /* Set to total force */
03099             for (ivc=0; ivc<3; ivc++) {
03100                 lforce[0].qfForce[ivc] +=
03101                     (scalar*Vunit_kb*(1e-3)*Vunit_Na*temp*aforce[0].qfForce[ivc]);
03102                 lforce[0].ibForce[ivc] +=
03103                     (scalar*Vunit_kb*(1e-3)*Vunit_Na*temp*aforce[0].ibForce[ivc]);
03104                 lforce[0].dbForce[ivc] +=
03105                     (scalar*Vunit_kb*(1e-3)*Vunit_Na*temp*aforce[0].dbForce[ivc]);
03106             }
03107         } else if (refcalcforce == PCF_COMPS) {
03108             for (ifr=0; ifr<refnforce; ifr++) {
03109                 for (ivc=0; ivc<3; ivc++) {
03110                     lforce[ifr].qfForce[ivc] +=
03111                         (scalar*Vunit_kb*(1e-3)*Vunit_Na*temp*aforce[ifr].qfForce[ivc]);
03112                     lforce[ifr].ibForce[ivc] +=
03113                         (scalar*Vunit_kb*(1e-3)*Vunit_Na*temp*aforce[ifr].ibForce[ivc]);
03114                     lforce[ifr].dbForce[ivc] +=
03115                         (scalar*Vunit_kb*(1e-3)*Vunit_Na*temp*aforce[ifr].dbForce[ivc]);
03116                 }
03117             }
03118         }
03119     }
03120
03121     Vnm_tprint( 0, "printEnergy: Performing global reduction (sum)\n");
03122     for (ifr=0; ifr<refnforce; ifr++) {
03123         Vcom_reduce(com, lforce[ifr].qfForce, gforce[ifr].qfForce, 3, 2, 0);
03124         Vcom_reduce(com, lforce[ifr].ibForce, gforce[ifr].ibForce, 3, 2, 0);
03125         Vcom_reduce(com, lforce[ifr].dbForce, gforce[ifr].dbForce, 3, 2, 0);
03126     }

```

```

03127
03128 #if 0
03129     if (refcalcforce == PCF_TOTAL) {
03130         Vnm_tprint( 1, " Local net fixed charge force = \
03131 (%1.12E, %1.12E, %1.12E) kJ/mol/A\n", lforce[0].qfForce[0],
03132 lforce[0].qfForce[1], lforce[0].qfForce[2]);
03133         Vnm_tprint( 1, " Local net ionic boundary force = \
03134 (%1.12E, %1.12E, %1.12E) kJ/mol/A\n", lforce[0].ibForce[0],
03135 lforce[0].ibForce[1], lforce[0].ibForce[2]);
03136         Vnm_tprint( 1, " Local net dielectric boundary force = \
03137 (%1.12E, %1.12E, %1.12E) kJ/mol/A\n", lforce[0].dbForce[0],
03138 lforce[0].dbForce[1], lforce[0].dbForce[2]);
03139     } else if (refcalcforce == PCF_COMPS) {
03140         for (ifr=0; ifr<refnforce; ifr++) {
03141             Vnm_tprint( 1, " Local fixed charge force \
03142 (atom %d) = (%1.12E, %1.12E, %1.12E) kJ/mol/A\n", ifr, lforce[ifr].qfForce[0],
03143 lforce[ifr].qfForce[1], lforce[ifr].qfForce[2]);
03144             Vnm_tprint( 1, " Local ionic boundary force \
03145 (atom %d) = (%1.12E, %1.12E, %1.12E) kJ/mol/A\n", ifr, lforce[ifr].ibForce[0],
03146 lforce[ifr].ibForce[1], lforce[ifr].ibForce[2]);
03147             Vnm_tprint( 1, " Local dielectric boundary force \
03148 (atom %d) = (%1.12E, %1.12E, %1.12E) kJ/mol/A\n", ifr, lforce[ifr].dbForce[0],
03149 lforce[ifr].dbForce[1], lforce[ifr].dbForce[2]);
03150         }
03151     }
03152 #endif
03153
03154     if (refcalcforce == PCF_TOTAL) {
03155         Vnm_tprint( 1, " Printing net forces (kJ/mol/A).\n");
03156         Vnm_tprint( 1, " Legend:\n");
03157         Vnm_tprint( 1, " tot -- Total force\n");
03158         Vnm_tprint( 1, " qf -- Fixed charge force\n");
03159         Vnm_tprint( 1, " db -- Dielectric boundary force\n");
03160         Vnm_tprint( 1, " ib -- Ionic boundary force\n");
03161
03162         for (ivc=0; ivc<3; ivc++) {
03163             totforce[ivc] =
03164 gforce[0].qfForce[ivc] + gforce[0].ibForce[ivc] \
03165 + gforce[0].dbForce[ivc];
03166         }
03167
03168         Vnm_tprint( 1, " tot %1.12E %1.12E %1.12E\n", totforce[0],
03169 totforce[1], totforce[2]);
03170         Vnm_tprint( 1, " qf %1.12E %1.12E %1.12E\n", gforce[0].qfForce[0],
03171 gforce[0].qfForce[1], gforce[0].qfForce[2]);
03172         Vnm_tprint( 1, " ib %1.12E %1.12E %1.12E\n", gforce[0].ibForce[0],
03173 gforce[0].ibForce[1], gforce[0].ibForce[2]);
03174         Vnm_tprint( 1, " db %1.12E %1.12E %1.12E\n", gforce[0].dbForce[0],
03175 gforce[0].dbForce[1], gforce[0].dbForce[2]);
03176
03177     } else if (refcalcforce == PCF_COMPS) {
03178
03179         Vnm_tprint( 1, " Printing per-atom forces (kJ/mol/A).\n");
03180         Vnm_tprint( 1, " Legend:\n");
03181         Vnm_tprint( 1, " tot n -- Total force for atom n\n");
03182         Vnm_tprint( 1, " qf n -- Fixed charge force for atom n\n");
03183         Vnm_tprint( 1, " db n -- Dielectric boundary force for atom n\n");
03184         Vnm_tprint( 1, " ib n -- Ionic boundary force for atom n\n");
03185         Vnm_tprint( 1, " tot all -- Total force for system\n");
03186
03187         totforce[0] = 0.0;
03188         totforce[1] = 0.0;
03189         totforce[2] = 0.0;
03190
03191         for (ifr=0; ifr<refnforce; ifr++) {
03192             Vnm_tprint( 1, " qf %d %1.12E %1.12E %1.12E\n", ifr,
03193 gforce[ifr].qfForce[0], gforce[ifr].qfForce[1],
03194 gforce[ifr].qfForce[2]);
03195             Vnm_tprint( 1, " ib %d %1.12E %1.12E %1.12E\n", ifr,
03196 gforce[ifr].ibForce[0], gforce[ifr].ibForce[1],
03197 gforce[ifr].ibForce[2]);
03198             Vnm_tprint( 1, " db %d %1.12E %1.12E %1.12E\n", ifr,
03199 gforce[ifr].dbForce[0], gforce[ifr].dbForce[1],
03200 gforce[ifr].dbForce[2]);
03201             Vnm_tprint( 1, " tot %d %1.12E %1.12E %1.12E\n", ifr,
03202 (gforce[ifr].dbForce[0] \
03203 + gforce[ifr].ibForce[0] +
03204 gforce[ifr].qfForce[0]),
03205 (gforce[ifr].dbForce[1] \
03206 + gforce[ifr].ibForce[1] +
03207 gforce[ifr].qfForce[1]),

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```

03208             (gforce[ifrc].dbForce[2] \
03209              + gforce[ifrc].ibForce[2] +
03210              gforce[ifrc].qfForce[2]));
03211     for (ivc=0; ivc<3; ivc++) {
03212         totforce[ivc] += (gforce[ifrc].dbForce[ivc] \
03213                          + gforce[ifrc].ibForce[ivc] \
03214                          + gforce[ifrc].qfForce[ivc]);
03215     }
03216 }
03217 Vnm_tprint( 1, " tot all %1.12E %1.12E %1.12E\n", totforce[0],
03218            totforce[1], totforce[2]);
03219 }
03220
03221 Vmem_free(VNULL, refnforce, sizeof(AtomForce), (void **>(&lforce));
03222 Vmem_free(VNULL, refnforce, sizeof(AtomForce), (void **>(&gforce));
03223
03224 return 1;
03225 }
03226 }
03227
03228 VPUBLIC int printElecForce(Vcom *com,
03229                          Nosh *nosh,
03230                          int nforce[NOSH_MAXCALC],
03231                          AtomForce *atomForce[NOSH_MAXCALC],
03232                          int iprint
03233                          ) {
03234
03235     int iarg,
03236         ifrc,
03237         ivc,
03238         calcid,
03239         refnforce,
03240         refcalcfrc;
03241     double temp,
03242         scalar,
03243         totforce[3];
03244     AtomForce *lforce, *gforce, *afrc;
03245
03246     if (Vstring_strcasecmp(nosh->elecname[nosh->printcalc[iprint][0]], "") == 0){
03247         Vnm_tprint( 1, "print force %d ", nosh->printcalc[iprint][0]+1);
03248     } else {
03249         Vnm_tprint( 1, "print force %d (%s) ", nosh->printcalc[iprint][0]+1,
03250                   nosh->elecname[nosh->printcalc[iprint][0]]);
03251     }
03252     for (iarg=1; iarg<nosh->printnarg[iprint]; iarg++) {
03253         if (nosh->printop[iprint][iarg-1] == 0)
03254             Vnm_tprint(1, "+ ");
03255         else if (nosh->printop[iprint][iarg-1] == 1)
03256             Vnm_tprint(1, "- ");
03257         else {
03258             Vnm_tprint( 2, "Undefined PRINT operation!\n");
03259             return 0;
03260         }
03261         if (Vstring_strcasecmp(nosh->elecname[nosh->printcalc[iprint][iarg]],
03262                               "") == 0) {
03263             Vnm_tprint( 1, "%d ", nosh->printcalc[iprint][iarg]+1);
03264         } else {
03265             Vnm_tprint( 1, "%d (%s) ", nosh->printcalc[iprint][iarg]+1,
03266                       nosh->elecname[nosh->printcalc[iprint][iarg]]);
03267         }
03268     }
03269     Vnm_tprint(1, "end\n");
03270
03271     /* First, go through and make sure we did the same type of force
03272      * evaluation in each of the requested calculations */
03273     calcid = nosh->elec2calc[nosh->printcalc[iprint][0]];
03274     refnforce = nforce[calcid];
03275     refcalcfrc = nosh->calc[calcid]->pbeparm->calcforce;
03276     if (refcalcfrc == PCF_NO) {
03277         Vnm_tprint( 2, " Didn't calculate force in calculation \
03278 %d\n", calcid+1);
03279         return 0;
03280     }
03281     for (iarg=1; iarg<nosh->printnarg[iprint]; iarg++) {
03282         calcid = nosh->elec2calc[nosh->printcalc[iprint][iarg]-1];
03283         if (nosh->calc[calcid]->pbeparm->calcforce != refcalcfrc) {
03284             Vnm_tprint(2, " Inconsistent calcforce declarations in \
03285 calculations %d and %d\n", nosh->elec2calc[nosh->printcalc[iprint][0]]+1,
03286                       calcid+1);
03287             return 0;
03288         }
03289     }

```

```

03289         if (nforce[calcid] != refnforce) {
03290             Vnm_tprint(2, " Inconsistent number of forces evaluated in \
03291 calculations %d and %d\n", nosh->elec2calc[nosh->printcalc[iprint][0]]+1,
03292                 calcid+1);
03293             return 0;
03294         }
03295     }
03296
03297     /* Now, allocate space to accumulate the forces */
03298     lforce = (AtomForce *)Vmem_malloc(VNULL, refnforce, sizeof(AtomForce));
03299     gforce = (AtomForce *)Vmem_malloc(VNULL, refnforce, sizeof(AtomForce));
03300
03301     /* Now, accumulate the forces */
03302     calcid = nosh->elec2calc[nosh->printcalc[iprint][0]];
03303     aforce = atomForce[calcid];
03304     temp = nosh->calc[calcid]->pbeparm->temp;
03305
03306     /* Load up the first calculation */
03307     if (refcalcforce == PCF_TOTAL) {
03308         /* Set to total force */
03309         for (ivc=0; ivc<3; ivc++) {
03310             lforce[0].qfForce[ivc] =
03311                 Vunit_kb*(1e-3)*Vunit_Na*temp*aforce[0].qfForce[ivc];
03312             lforce[0].ibForce[ivc] =
03313                 Vunit_kb*(1e-3)*Vunit_Na*temp*aforce[0].ibForce[ivc];
03314             lforce[0].dbForce[ivc] =
03315                 Vunit_kb*(1e-3)*Vunit_Na*temp*aforce[0].dbForce[ivc];
03316         }
03317     } else if (refcalcforce == PCF_COMPS) {
03318         for (ifr=0; ifr<refnforce; ifr++) {
03319             for (ivc=0; ivc<3; ivc++) {
03320                 lforce[ifr].qfForce[ivc] =
03321                     Vunit_kb*(1e-3)*Vunit_Na*temp*aforce[ifr].qfForce[ivc];
03322                 lforce[ifr].ibForce[ivc] =
03323                     Vunit_kb*(1e-3)*Vunit_Na*temp*aforce[ifr].ibForce[ivc];
03324                 lforce[ifr].dbForce[ivc] =
03325                     Vunit_kb*(1e-3)*Vunit_Na*temp*aforce[ifr].dbForce[ivc];
03326             }
03327         }
03328     }
03329
03330     /* Load up the rest of the calculations */
03331     for (iarg=1; iarg<nosh->printnarg[iprint]; iarg++) {
03332         calcid = nosh->elec2calc[nosh->printcalc[iprint][iarg]];
03333         temp = nosh->calc[calcid]->pbeparm->temp;
03334         aforce = atomForce[calcid];
03335         /* Get operation */
03336         if (nosh->printop[iprint][iarg-1] == 0) scalar = +1.0;
03337         else if (nosh->printop[iprint][iarg-1] == 1) scalar = -1.0;
03338         else scalar = 0.0;
03339         /* Accumulate */
03340         if (refcalcforce == PCF_TOTAL) {
03341             /* Set to total force */
03342             for (ivc=0; ivc<3; ivc++) {
03343                 lforce[0].qfForce[ivc] +=
03344                     (scalar*Vunit_kb*(1e-3)*Vunit_Na*temp*aforce[0].qfForce[ivc]);
03345                 lforce[0].ibForce[ivc] +=
03346                     (scalar*Vunit_kb*(1e-3)*Vunit_Na*temp*aforce[0].ibForce[ivc]);
03347                 lforce[0].dbForce[ivc] +=
03348                     (scalar*Vunit_kb*(1e-3)*Vunit_Na*temp*aforce[0].dbForce[ivc]);
03349             }
03350         } else if (refcalcforce == PCF_COMPS) {
03351             for (ifr=0; ifr<refnforce; ifr++) {
03352                 for (ivc=0; ivc<3; ivc++) {
03353                     lforce[ifr].qfForce[ivc] +=
03354                         (scalar*Vunit_kb*(1e-3)*Vunit_Na*temp*aforce[ifr].qfForce[ivc]);
03355                     lforce[ifr].ibForce[ivc] +=
03356                         (scalar*Vunit_kb*(1e-3)*Vunit_Na*temp*aforce[ifr].ibForce[ivc]);
03357                     lforce[ifr].dbForce[ivc] +=
03358                         (scalar*Vunit_kb*(1e-3)*Vunit_Na*temp*aforce[ifr].dbForce[ivc]);
03359                 }
03360             }
03361         }
03362     }
03363
03364     Vnm_tprint( 0, "printEnergy: Performing global reduction (sum)\n");
03365     for (ifr=0; ifr<refnforce; ifr++) {
03366         Vcom_reduce(com, lforce[ifr].qfForce, gforce[ifr].qfForce, 3, 2, 0);
03367         Vcom_reduce(com, lforce[ifr].ibForce, gforce[ifr].ibForce, 3, 2, 0);
03368         Vcom_reduce(com, lforce[ifr].dbForce, gforce[ifr].dbForce, 3, 2, 0);
03369     }

```

```

03370
03371 #if 0
03372     if (refcalcforce == PCF_TOTAL) {
03373         Vnm_tprint( 1, " Local net fixed charge force = \
03374 (%1.12E, %1.12E, %1.12E) kJ/mol/A\n", lforce[0].qfForce[0],
03375         lforce[0].qfForce[1], lforce[0].qfForce[2]);
03376         Vnm_tprint( 1, " Local net ionic boundary force = \
03377 (%1.12E, %1.12E, %1.12E) kJ/mol/A\n", lforce[0].ibForce[0],
03378         lforce[0].ibForce[1], lforce[0].ibForce[2]);
03379         Vnm_tprint( 1, " Local net dielectric boundary force = \
03380 (%1.12E, %1.12E, %1.12E) kJ/mol/A\n", lforce[0].dbForce[0],
03381         lforce[0].dbForce[1], lforce[0].dbForce[2]);
03382     } else if (refcalcforce == PCF_COMPS) {
03383         for (ifr=0; ifr<refnforce; ifr++) {
03384             Vnm_tprint( 1, " Local fixed charge force \
03385 (atom %d) = (%1.12E, %1.12E, %1.12E) kJ/mol/A\n", ifr, lforce[ifr].qfForce[0],
03386             lforce[ifr].qfForce[1], lforce[ifr].qfForce[2]);
03387             Vnm_tprint( 1, " Local ionic boundary force \
03388 (atom %d) = (%1.12E, %1.12E, %1.12E) kJ/mol/A\n", ifr, lforce[ifr].ibForce[0],
03389             lforce[ifr].ibForce[1], lforce[ifr].ibForce[2]);
03390             Vnm_tprint( 1, " Local dielectric boundary force \
03391 (atom %d) = (%1.12E, %1.12E, %1.12E) kJ/mol/A\n", ifr, lforce[ifr].dbForce[0],
03392             lforce[ifr].dbForce[1], lforce[ifr].dbForce[2]);
03393         }
03394     }
03395 #endif
03396
03397     if (refcalcforce == PCF_TOTAL) {
03398         Vnm_tprint( 1, " Printing net forces (kJ/mol/A).\n");
03399         Vnm_tprint( 1, " Legend:\n");
03400         Vnm_tprint( 1, " tot -- Total force\n");
03401         Vnm_tprint( 1, " qf -- Fixed charge force\n");
03402         Vnm_tprint( 1, " db -- Dielectric boundary force\n");
03403         Vnm_tprint( 1, " ib -- Ionic boundary force\n");
03404
03405         for (ivc=0; ivc<3; ivc++) {
03406             totforce[ivc] =
03407                 gforce[0].qfForce[ivc] + gforce[0].ibForce[ivc] \
03408                 + gforce[0].dbForce[ivc];
03409         }
03410
03411         Vnm_tprint( 1, " tot %1.12E %1.12E %1.12E\n", totforce[0],
03412             totforce[1], totforce[2]);
03413         Vnm_tprint( 1, " qf %1.12E %1.12E %1.12E\n", gforce[0].qfForce[0],
03414             gforce[0].qfForce[1], gforce[0].qfForce[2]);
03415         Vnm_tprint( 1, " ib %1.12E %1.12E %1.12E\n", gforce[0].ibForce[0],
03416             gforce[0].ibForce[1], gforce[0].ibForce[2]);
03417         Vnm_tprint( 1, " db %1.12E %1.12E %1.12E\n", gforce[0].dbForce[0],
03418             gforce[0].dbForce[1], gforce[0].dbForce[2]);
03419
03420     } else if (refcalcforce == PCF_COMPS) {
03421
03422         Vnm_tprint( 1, " Printing per-atom forces (kJ/mol/A).\n");
03423         Vnm_tprint( 1, " Legend:\n");
03424         Vnm_tprint( 1, " tot n -- Total force for atom n\n");
03425         Vnm_tprint( 1, " qf n -- Fixed charge force for atom n\n");
03426         Vnm_tprint( 1, " db n -- Dielectric boundary force for atom n\n");
03427         Vnm_tprint( 1, " ib n -- Ionic boundary force for atom n\n");
03428         Vnm_tprint( 1, " tot all -- Total force for system\n");
03429
03430         totforce[0] = 0.0;
03431         totforce[1] = 0.0;
03432         totforce[2] = 0.0;
03433
03434         for (ifr=0; ifr<refnforce; ifr++) {
03435             Vnm_tprint( 1, " qf %d %1.12E %1.12E %1.12E\n", ifr,
03436                 gforce[ifr].qfForce[0], gforce[ifr].qfForce[1],
03437                 gforce[ifr].qfForce[2]);
03438             Vnm_tprint( 1, " ib %d %1.12E %1.12E %1.12E\n", ifr,
03439                 gforce[ifr].ibForce[0], gforce[ifr].ibForce[1],
03440                 gforce[ifr].ibForce[2]);
03441             Vnm_tprint( 1, " db %d %1.12E %1.12E %1.12E\n", ifr,
03442                 gforce[ifr].dbForce[0], gforce[ifr].dbForce[1],
03443                 gforce[ifr].dbForce[2]);
03444             Vnm_tprint( 1, " tot %d %1.12E %1.12E %1.12E\n", ifr,
03445                 (gforce[ifr].dbForce[0] \
03446                 + gforce[ifr].ibForce[0] +
03447                 gforce[ifr].qfForce[0]),
03448                 (gforce[ifr].dbForce[1] \
03449                 + gforce[ifr].ibForce[1] +
03450                 gforce[ifr].qfForce[1]),

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03451         (gforce[ifrc].dbForce[2] \
03452          + gforce[ifrc].ibForce[2] +
03453          gforce[ifrc].qfForce[2]));
03454     for (ivc=0; ivc<3; ivc++) {
03455         totforce[ivc] += (gforce[ifrc].dbForce[ivc] \
03456                          + gforce[ifrc].ibForce[ivc] \
03457                          + gforce[ifrc].qfForce[ivc]);
03458     }
03459 }
03460 Vnm_tprint( 1, " tot all %1.12E %1.12E %1.12E\n", totforce[0],
03461            totforce[1], totforce[2]);
03462 }
03463
03464 Vmem_free(VNULL, refnforce, sizeof(AtomForce), (void **>(&lforce));
03465 Vmem_free(VNULL, refnforce, sizeof(AtomForce), (void **>(&gforce));
03466
03467 return 1;
03468
03469 }
03470
03471 VPUBLIC int printApolForce(Vcom *com,
03472                          Nosh *nosh,
03473                          int nforce[NOSH_MAXCALC],
03474                          AtomForce *atomForce[NOSH_MAXCALC],
03475                          int iprint
03476                          ) {
03477
03478     int iarg,
03479         ifrc,
03480         ivc,
03481         calcid,
03482         refnforce,
03483         refcalcforce;
03484     double temp,
03485         scalar,
03486         totforce[3];
03487     AtomForce *lforce,
03488              *gforce,
03489              *aforce;
03490
03491     if (Vstring_strcasecmp(nosh->apolname[nosh->printcalc[iprint][0]], "") == 0){
03492         Vnm_tprint( 1, "\nprint APOL force %d ", nosh->printcalc[iprint][0]+1);
03493     } else {
03494         Vnm_tprint( 1, "\nprint APOL force %d (%s) ", nosh->printcalc[iprint][0]+1,
03495                    nosh->apolname[nosh->printcalc[iprint][0]]);
03496     }
03497     for (iarg=1; iarg<nosh->printnarg[iprint]; iarg++) {
03498         if (nosh->printtop[iprint][iarg-1] == 0)
03499             Vnm_tprint(1, "+ ");
03500         else if (nosh->printtop[iprint][iarg-1] == 1)
03501             Vnm_tprint(1, "- ");
03502         else {
03503             Vnm_tprint( 2, "Undefined PRINT operation!\n");
03504             return 0;
03505         }
03506         if (Vstring_strcasecmp(nosh->apolname[nosh->printcalc[iprint][iarg]],
03507                                "") == 0) {
03508             Vnm_tprint( 1, "%d ", nosh->printcalc[iprint][iarg]+1);
03509         } else {
03510             Vnm_tprint( 1, "%d (%s) ", nosh->printcalc[iprint][iarg]+1,
03511                        nosh->apolname[nosh->printcalc[iprint][iarg]]);
03512         }
03513     }
03514     Vnm_tprint(1, "end\n");
03515
03516     /* First, go through and make sure we did the same type of force
03517      * evaluation in each of the requested calculations */
03518     calcid = nosh->apol2calc[nosh->printcalc[iprint][0]];
03519     refnforce = nforce[calcid];
03520     refcalcforce = nosh->calc[calcid]->apolparm->calcforce;
03521     if (refcalcforce == ACF_NO) {
03522         Vnm_tprint( 2, " Didn't calculate force in calculation \
03523 #%d\n", calcid+1);
03524         return 0;
03525     }
03526     for (iarg=1; iarg<nosh->printnarg[iprint]; iarg++) {
03527         calcid = nosh->apol2calc[nosh->printcalc[iprint][iarg]-1];
03528         if (nosh->calc[calcid]->apolparm->calcforce != refcalcforce) {
03529             Vnm_tprint(2, " Inconsistent calcforce declarations in \
03530 calculations %d and %d\n", nosh->apol2calc[nosh->printcalc[iprint][0]]+1,
03531                        calcid+1);

```

```

03532         return 0;
03533     }
03534     if (nforce[calcid] != refnforce) {
03535         Vnm_tprint(2, " Inconsistent number of forces evaluated in \
03536 calculations %d and %d\n", nosh->apol2calc[nosh->printcalc[iprint][0]]+1,
03537                 calcid+1);
03538         return 0;
03539     }
03540 }
03541
03542 /* Now, allocate space to accumulate the forces */
03543 lforce = (AtomForce *)Vmem_malloc(VNULL, refnforce, sizeof(AtomForce));
03544 gforce = (AtomForce *)Vmem_malloc(VNULL, refnforce, sizeof(AtomForce));
03545
03546 /* Now, accumulate the forces */
03547 calcid = nosh->apol2calc[nosh->printcalc[iprint][0]];
03548 aforce = atomForce[calcid];
03549 temp = nosh->calc[calcid]->apolparm->temp;
03550
03551 /* Load up the first calculation */
03552 if (refcalcforce == ACF_TOTAL) {
03553     /* Set to total force */
03554     for (ivc=0; ivc<3; ivc++) {
03555         lforce[0].sasaForce[ivc] = aforce[0].sasaForce[ivc];
03556         lforce[0].savForce[ivc] = aforce[0].savForce[ivc];
03557         lforce[0].wcaForce[ivc] = aforce[0].wcaForce[ivc];
03558     }
03559 } else if (refcalcforce == ACF_COMPS) {
03560     for (ifr=0; ifr<refnforce; ifr++) {
03561         for (ivc=0; ivc<3; ivc++) {
03562             lforce[ifr].sasaForce[ivc] = aforce[ifr].sasaForce[ivc];
03563             lforce[ifr].savForce[ivc] = aforce[ifr].savForce[ivc];
03564             lforce[ifr].wcaForce[ivc] = aforce[ifr].wcaForce[ivc];
03565         }
03566     }
03567 }
03568
03569 /* Load up the rest of the calculations */
03570 for (iarg=1; iarg<nosh->printnarg[iprint]; iarg++) {
03571     calcid = nosh->apol2calc[nosh->printcalc[iprint][iarg]];
03572     temp = nosh->calc[calcid]->apolparm->temp;
03573     aforce = atomForce[calcid];
03574     /* Get operation */
03575     if (nosh->printop[iprint][iarg-1] == 0) scalar = +1.0;
03576     else if (nosh->printop[iprint][iarg-1] == 1) scalar = -1.0;
03577     else scalar = 0.0;
03578     /* Accumulate */
03579     if (refcalcforce == ACF_TOTAL) {
03580         /* Set to total force */
03581         for (ivc=0; ivc<3; ivc++) {
03582             lforce[0].sasaForce[ivc] += aforce[0].sasaForce[ivc];
03583             lforce[0].savForce[ivc] += aforce[0].savForce[ivc];
03584             lforce[0].wcaForce[ivc] += aforce[0].wcaForce[ivc];
03585         }
03586     } else if (refcalcforce == ACF_COMPS) {
03587         for (ifr=0; ifr<refnforce; ifr++) {
03588             for (ivc=0; ivc<3; ivc++) {
03589                 lforce[ifr].sasaForce[ivc] += aforce[ifr].sasaForce[ivc];
03590                 lforce[ifr].savForce[ivc] += aforce[ifr].savForce[ivc];
03591                 lforce[ifr].wcaForce[ivc] += aforce[ifr].wcaForce[ivc];
03592             }
03593         }
03594     }
03595 }
03596
03597 Vnm_tprint( 0, "printForce: Performing global reduction (sum)\n");
03598 for (ifr=0; ifr<refnforce; ifr++) {
03599     Vcom_reduce(com, lforce[ifr].sasaForce, gforce[ifr].sasaForce, 3, 2, 0);
03600     Vcom_reduce(com, lforce[ifr].savForce, gforce[ifr].savForce, 3, 2, 0);
03601     Vcom_reduce(com, lforce[ifr].wcaForce, gforce[ifr].wcaForce, 3, 2, 0);
03602 }
03603
03604 if (refcalcforce == ACF_TOTAL) {
03605     Vnm_tprint( 1, " Printing net forces (kJ/mol/A)\n");
03606     Vnm_tprint( 1, " Legend:\n");
03607     Vnm_tprint( 1, " tot -- Total force\n");
03608     Vnm_tprint( 1, " sasa -- SASA force\n");
03609     Vnm_tprint( 1, " sav -- SAV force\n");
03610     Vnm_tprint( 1, " wca -- WCA force\n\n");
03611
03612     for (ivc=0; ivc<3; ivc++) {

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03613         totforce[ivc] =
03614         gforce[0].sasaForce[ivc] + gforce[0].savForce[ivc] \
03615         + gforce[0].wcaForce[ivc];
03616     }
03617
03618     Vnm_tprint( 1, " tot %1.12E %1.12E %1.12E\n", totforce[0],
03619               totforce[1], totforce[2]);
03620     Vnm_tprint( 1, " sasa %1.12E %1.12E %1.12E\n", gforce[0].sasaForce[0],
03621               gforce[0].sasaForce[1], gforce[0].sasaForce[2]);
03622     Vnm_tprint( 1, " sav %1.12E %1.12E %1.12E\n", gforce[0].savForce[0],
03623               gforce[0].savForce[1], gforce[0].savForce[2]);
03624     Vnm_tprint( 1, " wca %1.12E %1.12E %1.12E\n", gforce[0].wcaForce[0],
03625               gforce[0].wcaForce[1], gforce[0].wcaForce[2]);
03626
03627     } else if (refcalcforce == ACF_COMPS) {
03628
03629         Vnm_tprint( 1, " Printing per atom forces (kJ/mol/A)\n");
03630         Vnm_tprint( 1, " Legend:\n");
03631         Vnm_tprint( 1, " tot n -- Total force for atom n\n");
03632         Vnm_tprint( 1, " sasa n -- SASA force for atom n\n");
03633         Vnm_tprint( 1, " sav n -- SAV force for atom n\n");
03634         Vnm_tprint( 1, " wca n -- WCA force for atom n\n");
03635         Vnm_tprint( 1, " tot all -- Total force for system\n");
03636
03637         //Vnm_tprint( 1, " gamma, pressure, bconc are: %f %f %f\n",
03638         //          gamma,press,bconc);
03639
03640         totforce[0] = 0.0;
03641         totforce[1] = 0.0;
03642         totforce[2] = 0.0;
03643
03644         for (ifr=0; ifr<refnforce; ifr++) {
03645             Vnm_tprint( 1, " sasa %d %1.12E %1.12E %1.12E\n", ifr,
03646                       gforce[ifr].sasaForce[0], gforce[ifr].sasaForce[1],
03647                       gforce[ifr].sasaForce[2]);
03648             Vnm_tprint( 1, " sav %d %1.12E %1.12E %1.12E\n", ifr,
03649                       gforce[ifr].savForce[0], gforce[ifr].savForce[1],
03650                       gforce[ifr].savForce[2]);
03651             Vnm_tprint( 1, " wca %d %1.12E %1.12E %1.12E\n", ifr,
03652                       gforce[ifr].wcaForce[0], gforce[ifr].wcaForce[1],
03653                       gforce[ifr].wcaForce[2]);
03654             Vnm_tprint( 1, " tot %d %1.12E %1.12E %1.12E\n", ifr,
03655                       (gforce[ifr].wcaForce[0] \
03656                        + gforce[ifr].savForce[0] +
03657                        gforce[ifr].sasaForce[0]),
03658                       (gforce[ifr].wcaForce[1] \
03659                        + gforce[ifr].savForce[1] +
03660                        gforce[ifr].sasaForce[1]),
03661                       (gforce[ifr].wcaForce[2] \
03662                        + gforce[ifr].savForce[2] +
03663                        gforce[ifr].sasaForce[2]));
03664             for (ivc=0; ivc<3; ivc++) {
03665                 totforce[ivc] += (gforce[ifr].wcaForce[ivc] \
03666                                   + gforce[ifr].savForce[ivc] \
03667                                   + gforce[ifr].sasaForce[ivc]);
03668             }
03669         }
03670         Vnm_tprint( 1, " tot all %1.12E %1.12E %1.12E\n", totforce[0],
03671               totforce[1], totforce[2]);
03672     }
03673
03674     Vmem_free(VNULL, refnforce, sizeof(AtomForce), (void **)(&lforce));
03675     Vmem_free(VNULL, refnforce, sizeof(AtomForce), (void **)(&gforce));
03676
03677     return 1;
03678 }
03679
03680 #ifdef HAVE_MC_H
03681
03682
03683 VPUBLIC void killFE(NOsh *nosh,
03684                   Vpbe *pbe[NOSH_MAXCALC],
03685                   Vfetc *fetc[NOSH_MAXCALC],
03686                   Gem *gm[NOSH_MAXMOL]
03687                   ) {
03688
03689     int i;
03690
03691 #ifndef VAPBSQUIET
03692     Vnm_tprint(1, "Destroying finite element structures.\n");
03693 #endif

```

```

03694
03695     for(i=0;i<nosh->ncalc;i++){
03696         Vpbe_dtor(&(pbe[i]));
03697         Vfetc_dtor(&(fetc[i]));
03698     }
03699     for (i=0; i<nosh->nmesh; i++) {
03700         Gem_dtor(&(gm[i]));
03701     }
03702 }
03703
03711 VPUBLIC Vrc_Codes initFE(int icalc,
03712                         Nosh *nosh,
03713                         FEMparm *feparm,
03714                         PBEparm *pbeparm,
03715                         Vpbe *pbe[NOSH_MAXCALC],
03716                         Valist *alist[NOSH_MAXMOL],
03717                         Vfetc *fetc[NOSH_MAXCALC]
03718     ) {
03719
03720     int iatom,
03721         imesh,
03722         i,
03723         j,
03724         theMol,
03725         focusFlag = 0;
03726     Vio *sock = VNULL;
03727     size_t bytesTotal,
03728           highWater;
03729     Vfetc_MeshLoad meshType;
03730     double length[3],
03731           center[3],
03732           sparm,
03733           q,
03734           iparm = 0.0;
03735     Vrc_Codes vrc;
03736     Valist *myalist;
03737     Vatom *atom = VNULL;
03738     Vnm_tstart(27, "Setup timer");
03739
03740
03741     /* Print some warning messages */
03742     if (pbeparm->useDielMap) Vnm_tprint(2, "FEM ignoring dielectric map!\n");
03743     if (pbeparm->useKappaMap) Vnm_tprint(2, "FEM ignoring kappa map!\n");
03744     if (pbeparm->useChargeMap) Vnm_tprint(2, "FEM ignoring charge map!\n");
03745
03746     /* Fix mesh center for "GCENT MOL #" types of declarations. */
03747     Vnm_tprint(0, "Re-centering mesh...\n");
03748     theMol = pbeparm->molid-1;
03749     myalist = alist[theMol];
03750     for (j=0; j<3; j++) {
03751         if (theMol < nosh->nmol) {
03752             center[j] = (myalist->center[j]);
03753         } else{
03754             Vnm_tprint(2, "ERROR! Bogus molecule number (%d)!\n",
03755                       (theMol+1));
03756             return VRC_FAILURE;
03757         }
03758     }
03759
03760     /* Check for completely-neutral molecule */
03761     q = 0;
03762     for (iatom=0; iatom<Valist_getNumberAtoms(myalist); iatom++) {
03763         atom = Valist_getAtom(myalist, iatom);
03764         q += VSQR(Vatom_getCharge(atom));
03765     }
03766     /* D. Gohara 10/22/09 - disabled
03767     if (q < (1e-6)) {
03768         Vnm_tprint(2, "Molecule #%d is uncharged!\n", pbeparm->molid);
03769         Vnm_tprint(2, "Sum square charge = %g!\n", q);
03770         return VRC_FAILURE;
03771     }
03772     */
03773
03774     /* Set the feparm pkey value based on the presence of an HB solver */
03775     #ifdef USE_HB
03776         feparm->pkey = 1;
03777     #else
03778         feparm->pkey = 0;
03779     #endif
03780
03781     /* Set up PBE object */
03782     Vnm_tprint(0, "Setting up PBE object...\n");

```

```
03783     if (pbeparm->srfm == VSM_SPLINE) {
03784         sparm = pbeparm->swin;
03785     }
03786     else {
03787         sparm = pbeparm->srاد;
03788     }
03789     if (pbeparm->nion > 0) {
03790         iparm = pbeparm->ionr[0];
03791     }
03792
03793     pbe[icalc] = Vpbe_ctor(myalist, pbeparm->nion,
03794         pbeparm->ionc, pbeparm->ionr, pbeparm->ionq,
03795         pbeparm->temp, pbeparm->pdie,
03796         pbeparm->sdie, sparm, focusFlag, pbeparm->sdens,
03797         pbeparm->zmem, pbeparm->Lmem, pbeparm->mdie,
03798         pbeparm->memv);
03799
03800     /* Print a few derived parameters */
03801     Vnm_tprint(1, " Debye length:  %g A\n", Vpbe_getDeblen(pbe[icalc]));
03802
03803     /* Set up FEtk objects */
03804     Vnm_tprint(0, "Setting up FEtk object...\n");
03805     fetk[icalc] = Vfetk_ctor(pbe[icalc], pbeparm->pbetype);
03806     Vfetk_setParameters(fetk[icalc], pbeparm, feparm);
03807
03808     /* Build mesh - this merely loads an MCSF file from an external source if one is specified or uses the
03809      * current molecule and sets center/length values based on that molecule if no external source is
03810      * specified. */
03811     Vnm_tprint(0, "Setting up mesh...\n");
03812     sock = VNULL;
03813     if (feparm->useMesh) {
03814         imesh = feparm->meshID-1;
03815         meshType = VML_EXTERNAL;
03816         for (i=0; i<3; i++) {
03817             center[i] = 0.0;
03818             length[i] = 0.0;
03819         }
03820         Vnm_print(0, "Using mesh %d (%s) in calculation.\n", imesh+1,
03821             nosh->meshpath[imesh]);
03822         switch (nosh->meshfmt[imesh]) {
03823             case VDF_DX:
03824                 Vnm_tprint(2, "DX finite element mesh input not supported yet!\n");
03825                 return VRC_FAILURE;
03826             case VDF_DXBIN:
03827                 Vnm_tprint(2, "DXBIN finite element mesh input not supported yet!\n");
03828                 return VRC_FAILURE;
03829             case VDF_UHBD:
03830                 Vnm_tprint( 2, "UHBD finite element mesh input not supported!\n");
03831                 return VRC_FAILURE;
03832             case VDF_AVS:
03833                 Vnm_tprint( 2, "AVS finite element mesh input not supported!\n");
03834                 return VRC_FAILURE;
03835             case VDF_MCSF:
03836                 Vnm_tprint(1, "Reading MCSF-format input finite element mesh from %s.\n",
03837                     nosh->meshpath[imesh]);
03838                 sock = Vio_ctor("FILE", "ASC", VNULL, nosh->meshpath[imesh], "r");
03839                 if (sock == VNULL) {
03840                     Vnm_print(2, "Problem opening virtual socket %s!\n",
03841                         nosh->meshpath[imesh]);
03842                     return VRC_FAILURE;
03843                 }
03844                 if (Vio_accept(sock, 0) < 0) {
03845                     Vnm_print(2, "Problem accepting virtual socket %s!\n",
03846                         nosh->meshpath[imesh]);
03847                     return VRC_FAILURE;
03848                 }
03849                 break;
03850             default:
03851                 Vnm_tprint( 2, "Invalid data format (%d)!\n",
03852                     nosh->meshfmt[imesh]);
03853                 return VRC_FAILURE;
03854         }
03855     }
03856     else { /* if (feparm->useMesh) */
03857         meshType = VML_DIRICUBE;
03858         for (i=0; i<3; i++) {
03859             center[i] = alist[theMol]->center[i];
03860             length[i] = feparm->glen[i];
03861         }
03862     }
03863 }
```

```

03864      /* Load the mesh with a particular center and vertex length using the provided input socket */
03865      vrc = Vfetk_loadMesh(fetk[icalc], center, length, meshType, sock);
03866      if (vrc == VRC_FAILURE) {
03867          Vnm_print(2, "Error constructing finite element mesh!\n");
03868          return VRC_FAILURE;
03869      }
03870      //Vnm_redirect(0); // Redirect output to io.mc
03871      Gem_shapeChk(fetk[icalc]->gm); // Traverse simplices and check shapes using the geometry manager.
03872      //Vnm_redirect(1);
03873
03874      /* Uniformly refine the mesh a bit */
03875      for (j=0; j<2; j++) {
03876          /* AM_* calls below are from the MC package, mc/src/nam/am.c. Note that these calls actually are
03877           * wrappers around Aprx_* functions found in MC as well. */
03878          /* Mark the mesh for needed refinements */
03879          AM_markRefine(fetk[icalc]->am, 0, -1, 0, 0.0);
03880          /* Do actual mesh refinement */
03881          AM_refine(fetk[icalc]->am, 2, 0, feparm->pkey);
03882          //Vnm_redirect(0); // Redirect output to io.mc
03883          Gem_shapeChk(fetk[icalc]->gm); // Traverse simplices and check shapes using the geometry manager.
03884          //Vnm_redirect(1);
03885      }
03886
03887      /* Setup time statistics */
03888      Vnm_tstop(27, "Setup timer");
03889
03890      /* Memory statistics */
03891      bytesTotal = Vmem_bytesTotal();
03892      highWater = Vmem_highWaterTotal();
03893
03894      #ifndef VAPBSQUIET
03895          Vnm_tprint(1, " Current memory usage: %4.3f MB total, \
03896          %4.3f MB high water\n", (double)(bytesTotal)/(1024.*1024.),
03897          (double)(highWater)/(1024.*1024.));
03898      #endif
03899
03900      return VRC_SUCCESS;
03901  }
03902
03903  VPUBLIC void printFEPARM(int icalc,
03904                          NOsh *nosh,
03905                          FEParm *feparm,
03906                          Vfetk *fetk[NOSH_MAXCALC]
03907                          ) {
03908
03909      Vnm_tprint(1, " Domain size: %g A x %g A x %g A\n",
03910                  feparm->glen[0], feparm->glen[1],
03911                  feparm->glen[2]);
03912      switch(feparm->ekey) {
03913          case FET_SIMP:
03914              Vnm_tprint(1, " Per-simplex error tolerance: %g\n", feparm->etol);
03915              break;
03916          case FET_GLOB:
03917              Vnm_tprint(1, " Global error tolerance: %g\n", feparm->etol);
03918              break;
03919          case FET_FRAC:
03920              Vnm_tprint(1, " Fraction of simp to refine: %g\n", feparm->etol);
03921              break;
03922          default:
03923              Vnm_tprint(2, "Invalid ekey (%d)!\n", feparm->ekey);
03924              VASSERT(0);
03925              break;
03926      }
03927      switch(feparm->akeyPRE) {
03928          case FRT_UNIF:
03929              Vnm_tprint(1, " Uniform pre-solve refinement.\n");
03930              break;
03931          case FRT_GEOM:
03932              Vnm_tprint(1, " Geometry-based pre-solve refinement.\n");
03933              break;
03934          default:
03935              Vnm_tprint(2, "Invalid akeyPRE (%d)!\n", feparm->akeyPRE);
03936              VASSERT(0);
03937              break;
03938      }
03939      switch(feparm->akeySOLVE) {
03940          case FRT_RESI:
03941              Vnm_tprint(1, " Residual-based a posteriori refinement.\n");
03942              break;
03943          case FRT_DUAL:
03944              Vnm_tprint(1, " Dual-based a posteriori refinement.\n");

```

```

03945         break;
03946     case FRT_LOCA:
03947         Vnm_tprint(1, " Local-based a posteriori refinement.\n");
03948         break;
03949     default:
03950         Vnm_tprint(2, "Invalid akeySOLVE (%d)!\n", feparm->akeySOLVE);
03951         break;
03952 }
03953 Vnm_tprint(1, " Refinement of initial mesh to ~%d vertices\n",
03954           feparm->targetNum);
03955 Vnm_tprint(1, " Geometry-based refinement lower bound: %g A\n",
03956           feparm->targetRes);
03957 Vnm_tprint(1, " Maximum number of solve-estimate-refine cycles: %d\n",
03958           feparm->maxsolve);
03959 Vnm_tprint(1, " Maximum number of vertices in mesh: %d\n",
03960           feparm->maxvert);
03961
03962 /* FOLLOWING IS SOLVER-RELATED; BAIL IF NOT SOLVING */
03963 if (nosh->bogus) return;
03964 #ifdef USE_HB
03965     Vnm_tprint(1, " HB linear solver: AM_hPcg\n");
03966 #else
03967     Vnm_tprint(1, " Non-HB linear solver: ");
03968     switch (fetk[icalc]->lkey) {
03969     case VLT_SLU:
03970         Vnm_print(1, "SLU direct\n");
03971         break;
03972     case VLT_MG:
03973         Vnm_print(1, "multigrid\n");
03974         break;
03975     case VLT_CG:
03976         Vnm_print(1, "conjugate gradient\n");
03977         break;
03978     case VLT_BCG:
03979         Vnm_print(1, "BiCGStab\n");
03980         break;
03981     default:
03982         Vnm_print(1, "???\n");
03983         break;
03984     }
03985 #endif
03986
03987 Vnm_tprint(1, " Linear solver tol.: %g\n", fetk[icalc]->ltol);
03988 Vnm_tprint(1, " Linear solver max. iters.: %d\n", fetk[icalc]->lmax);
03989 Vnm_tprint(1, " Linear solver preconditioner: ");
03990 switch (fetk[icalc]->lprec) {
03991 case VPT_IDEN:
03992     Vnm_print(1, "identity\n");
03993     break;
03994 case VPT_DIAG:
03995     Vnm_print(1, "diagonal\n");
03996     break;
03997 case VPT_MG:
03998     Vnm_print(1, "multigrid\n");
03999     break;
04000 default:
04001     Vnm_print(1, "???\n");
04002     break;
04003 }
04004 Vnm_tprint(1, " Nonlinear solver: ");
04005 switch (fetk[icalc]->nkey) {
04006 case VNT_NEW:
04007     Vnm_print(1, "newton\n");
04008     break;
04009 case VNT_INC:
04010     Vnm_print(1, "incremental\n");
04011     break;
04012 case VNT_ARC:
04013     Vnm_print(1, "pseudo-arclength\n");
04014     break;
04015 default:
04016     Vnm_print(1, "??? ");
04017     break;
04018 }
04019 Vnm_tprint(1, " Nonlinear solver tol.: %g\n", fetk[icalc]->ntol);
04020 Vnm_tprint(1, " Nonlinear solver max. iters.: %d\n", fetk[icalc]->nmax);
04021 Vnm_tprint(1, " Initial guess: ");
04022 switch (fetk[icalc]->gues) {
04023 case VGT_ZERO:
04024     Vnm_tprint(1, "zero\n");
04025     break;

```

```

04026         case VGT_DIRI:
04027             Vnm_tprint(1, "boundary function\n");
04028             break;
04029         case VGT_PREV:
04030             Vnm_tprint(1, "interpolated previous solution\n");
04031             break;
04032         default:
04033             Vnm_tprint(1, "???\n");
04034             break;
04035     }
04036 }
04037 }
04038
04039 VPUBLIC int partFE(int icalc, NOsh *nosh, FEMparm *feparm,
04040                  Vfetk *fetk[NOSH_MAXCALC]) {
04041
04042     Vfetk_setAtomColors(fetk[icalc]);
04043     return 1;
04044 }
04045
04046 VPUBLIC int preRefineFE(int icalc, /* Calculation index */
04047                      FEMparm *feparm, /* FE-specific parameters */
04048                      Vfetk *fetk[NOSH_MAXCALC] /* Array of FE solver objects */
04049                      ) {
04050
04051     int nverts,
04052         marked;
04053     /* Based on the refinement type, alert the user to what we're trying to refine with. */
04054     switch(feparm->akeyPRE) {
04055     case FRT_UNIF:
04056         Vnm_tprint(1, " Commencing uniform refinement to %d verts.\n",
04057                  feparm->targetNum);
04058         break;
04059     case FRT_GEOM:
04060         Vnm_tprint(1, " Commencing geometry-based refinement to %d \
04061         verts or %g A resolution.\n", feparm->targetNum, feparm->targetRes);
04062         break;
04063     case FRT_DUAL:
04064         Vnm_tprint(2, "What? You can't do a posteriori error estimation \
04065         before you solve!\n");
04066         VASSERT(0);
04067         break;
04068     case FRT_RESI:
04069     case FRT_LOCA:
04070     default:
04071         VASSERT(0);
04072         break;
04073     }
04074
04075     Vnm_tprint(1, " Initial mesh has %d vertices\n",
04076              Gem_numVV(fetk[icalc]->gm));
04077
04078     /* As long as we have simplices marked that need to be refined, run MC's
04079     * AM_markRefine against our data until we hit the error or size tolerance
04080     * for the refinement. */
04081     while (1) {
04082         nverts = Gem_numVV(fetk[icalc]->gm);
04083         if (nverts > feparm->targetNum) {
04084             Vnm_tprint(1, " Hit vertex number limit.\n");
04085             break;
04086         }
04087         marked = AM_markRefine(fetk[icalc]->am, feparm->akeyPRE, -1,
04088                              feparm->ekey, feparm->etol);
04089         if (marked == 0) {
04090             Vnm_tprint(1, " Marked 0 sims; hit error/size tolerance.\n");
04091             break;
04092         }
04093         Vnm_tprint(1, " Have %d verts, marked %d. Refining...\n", nverts,
04094                  marked);
04095         AM_refine(fetk[icalc]->am, 0, 0, feparm->pkey);
04096     }
04097
04098     nverts = Gem_numVV(fetk[icalc]->gm);
04099     Vnm_tprint(1, " Done refining; have %d verts.\n", nverts);
04100
04101     return 1;
04102 }
04103
04104 VPUBLIC int solveFE(int icalc,
04105                   PBEParm *pbeparm,

```



```

04118             FEMparm *feparm,
04119             Vfetk *fetk[NOSH_MAXCALC]
04120         ) {
04121
04122         int lkeyHB = 3,
04123             meth = 2,
04124             prob = 0,
04125             prec = 0;
04126
04127         if ((pbeparm->pbetype==PBE_NPBE) ||
04128             (pbeparm->pbetype == PBE_NRPBE) ||
04129             (pbeparm->pbetype == PBE_SMPBE)) {
04130
04131             /* Call MC's nonlinear solver - mc/src/nam/nsolv.c */
04132             AM_nSolve(
04133                 fetk[icalc]->am,
04134                 fetk[icalc]->nkey,
04135                 fetk[icalc]->nmax,
04136                 fetk[icalc]->ntol,
04137                 meth,
04138                 fetk[icalc]->lmax,
04139                 fetk[icalc]->ltol,
04140                 prec,
04141                 fetk[icalc]->gues,
04142                 fetk[icalc]->pjac
04143             );
04144         } else if ((pbeparm->pbetype==PBE_LPBE) ||
04145                 (pbeparm->pbetype==PBE_LRPBE)) {
04146             /* Note: USEHB is a compile time defined macro. The program flow
04147              is to always take the route using AM_hlSolve when the solver
04148              is linear. D. Gohara 6/29/06
04149              */
04150             #ifdef USE_HB
04151                 Vnm_print(2, "SORRY! DON'T USE HB!!!\n");
04152                 VASSERT(0);
04153             #endif
04154
04155             /* Call MC's hierarchical linear solver - mc/src/nam/lsolv.c */
04156             AM_hlSolve(fetk[icalc]->am, meth, lkeyHB, fetk[icalc]->lmax,
04157                       fetk[icalc]->ltol, fetk[icalc]->gues, fetk[icalc]->pjac);
04158         } else
04159             /* Call MC's linear solver - mc/src/nam/lsolv.c */
04160             AM_lSolve(
04161                 fetk[icalc]->am,
04162                 prob,
04163                 meth,
04164                 fetk[icalc]->lmax,
04165                 fetk[icalc]->ltol,
04166                 prec,
04167                 fetk[icalc]->gues,
04168                 fetk[icalc]->pjac
04169             );
04170         #endif
04171     }
04172     return 1;
04173 }
04174
04175 VPUBLIC int energyFE(Nosh *nosh,
04176                     int icalc,
04177                     Vfetk *fetk[NOSH_MAXCALC],
04178                     int *nenergy,
04179                     double *totEnergy,
04180                     double *qfEnergy,
04181                     double *qmEnergy,
04182                     double *dielEnergy
04183                 ) {
04184
04185     FEMparm *feparm = nosh->calc[icalc]->feparm;
04186     PBEparm *pbeparm = nosh->calc[icalc]->pbeparm;
04187     *nenergy = 1;
04188     *totEnergy = 0;
04189
04190     if (nosh->bogus == 0) {
04191         if ((pbeparm->pbetype==PBE_NPBE) ||
04192             (pbeparm->pbetype==PBE_NRPBE) ||
04193             (pbeparm->pbetype == PBE_SMPBE)) {
04194             *totEnergy = Vfetk_energy(fetk[icalc], -1, 1); /* Last parameter indicates NPBE */
04195         } else if ((pbeparm->pbetype==PBE_LPBE) ||
04196                 (pbeparm->pbetype==PBE_LRPBE)) {
04197             *totEnergy = Vfetk_energy(fetk[icalc], -1, 0); /* Last parameter indicates LPBE */
04198         } else {

```

```

04210         VASSERT(0);
04211     }
04212
04213 #ifndef VAPBSQUIET
04214     Vnm_tprint(1, "        Total electrostatic energy = %1.12E kJ/mol\n",
04215         Vunit_kb*pbeParm->temp*(1e-3)*Vunit_Na*(totEnergy));
04216     fflush(stdout);
04217 #endif
04218 }
04219
04220 if (pbeParm->calcEnergy == PCE_COMPS) {
04221     Vnm_tprint(2, "Error!  Verbose energy evaluation not available for FEM yet!\n");
04222     Vnm_tprint(2, "E-mail nathan.baker@pnl.gov if you want this.\n");
04223     *qfEnergy = 0;
04224     *qmEnergy = 0;
04225     *dielEnergy = 0;
04226 } else {
04227     *nenergy = 0;
04228 }
04229 return 1;
04230 }
04231
04232 VPUBLIC int postRefineFE(int icalc,
04233     FEMparm *feparm,
04234     Vfetc *fetc[NOSH_MAXCALC]
04235 ) {
04236
04237     int nverts,
04238         marked;
04239     nverts = Gem_numVV(fetc[icalc]->gm);
04240     if (nverts > feparm->maxvert) {
04241         Vnm_tprint(1, "        Current number of vertices (%d) exceeds max (%d)!\n",
04242             nverts, feparm->maxvert);
04243         return 0;
04244     }
04245     Vnm_tprint(1, "        Mesh currently has %d vertices\n", nverts);
04246
04247     switch(feparm->aKeySOLVE) {
04248     case FRT_UNIF:
04249         Vnm_tprint(1, "        Commencing uniform refinement.\n");
04250         break;
04251     case FRT_GEOM:
04252         Vnm_tprint(1, "        Commencing geometry-based refinement.\n");
04253         break;
04254     case FRT_RESI:
04255         Vnm_tprint(1, "        Commencing residual-based refinement.\n");
04256         break;
04257     case FRT_DUAL:
04258         Vnm_tprint(1, "        Commencing dual problem-based refinement.\n");
04259         break;
04260     case FRT_LOCA:
04261         Vnm_tprint(1, "        Commencing local-based refinement.\n");
04262         break;
04263     default:
04264         Vnm_tprint(2, "        Error -- unknown refinement type (%d)!\n",
04265             feparm->aKeySOLVE);
04266         return 0;
04267         break;
04268     }
04269
04270     /* Run MC's refinement algorithm */
04271     marked = AM_markRefine(fetc[icalc]->am, feparm->aKeySOLVE, -1,
04272         feparm->eKey, feparm->etol);
04273     if (marked == 0) {
04274         Vnm_tprint(1, "        Marked 0 sims; hit error/size tolerance.\n");
04275         return 0;
04276     }
04277     Vnm_tprint(1, "        Have %d verts, marked %d.  Refining...\n", nverts,
04278         marked);
04279     AM_refine(fetc[icalc]->am, 0, 0, feparm->pKey);
04280     nverts = Gem_numVV(fetc[icalc]->gm);
04281     Vnm_tprint(1, "        Done refining; have %d verts.\n", nverts);
04282     //Vnm_redirect(0); // Redirect output to io.mc
04283     Gem_shapeChk(fetc[icalc]->gm); // Traverse simplices and check shapes using the geometry manager.
04284     //Vnm_redirect(1);
04285
04286     return 1;
04287 }
04288
04289 VPUBLIC int writedataFE(int rank,
04290     Nosh *nosh,

```

```
04302             PBEParm *pbeparm,
04303             Vfetk *fetk
04304         ) {
04305
04306         char writestem[VMAX_ARGLEN];
04307         char outpath[VMAX_ARGLEN];
04308         int i,
04309             writeit;
04310         AM *am;
04311         Bvec *vec;
04312         if (nosh->bogus) return 1;
04313
04314         am = fetk->am;
04315         vec = am->w0;
04316
04317         for (i=0; i<pbeparm->numwrite; i++) {
04318
04319             writeit = 1;
04320
04321             switch (pbeparm->writetype[i]) {
04322
04323                 case VDT_CHARGE:
04324
04325                     Vnm_tprint(2, "      Sorry; can't write charge distribution for FEM!\n");
04326                     writeit = 0;
04327                     break;
04328
04329                 case VDT_POT:
04330
04331                     Vnm_tprint(1, "      Writing potential to ");
04332                     Vfetk_fillArray(fetk, vec, VDT_POT);
04333                     break;
04334
04335                 case VDT_SMOL:
04336
04337                     Vnm_tprint(1, "      Writing molecular accessibility to ");
04338                     Vfetk_fillArray(fetk, vec, VDT_SMOL);
04339                     break;
04340
04341                 case VDT_SSPL:
04342
04343                     Vnm_tprint(1, "      Writing spline-based accessibility to ");
04344                     Vfetk_fillArray(fetk, vec, VDT_SSPL);
04345                     break;
04346
04347                 case VDT_VDW:
04348
04349                     Vnm_tprint(1, "      Writing van der Waals accessibility to ");
04350                     Vfetk_fillArray(fetk, vec, VDT_VDW);
04351                     break;
04352
04353                 case VDT_IVDW:
04354
04355                     Vnm_tprint(1, "      Writing ion accessibility to ");
04356                     Vfetk_fillArray(fetk, vec, VDT_IVDW);
04357                     break;
04358
04359                 case VDT_LAP:
04360
04361                     Vnm_tprint(2, "      Sorry; can't write charge distribution for FEM!\n");
04362                     writeit = 0;
04363                     break;
04364
04365                 case VDT_EDENS:
04366
04367                     Vnm_tprint(2, "      Sorry; can't write energy density for FEM!\n");
04368                     writeit = 0;
04369                     break;
04370
04371                 case VDT_NDENS:
04372
04373                     Vnm_tprint(1, "      Writing number density to ");
04374                     Vfetk_fillArray(fetk, vec, VDT_NDENS);
04375                     break;
04376
04377                 case VDT_QDENS:
04378
04379                     Vnm_tprint(1, "      Writing charge density to ");
04380                     Vfetk_fillArray(fetk, vec, VDT_QDENS);
04381                     break;
04382
04383             }
```

```

04384         case VDT_DIELX:
04385
04386             Vnm_tprint(2, "    Sorry; can't write x-shifted dielectric map for FEM!\n");
04387             writeit = 0;
04388             break;
04389
04390         case VDT_DIELY:
04391
04392             Vnm_tprint(2, "    Sorry; can't write y-shifted dielectric map for FEM!\n");
04393             writeit = 0;
04394             break;
04395
04396         case VDT_DIELZ:
04397
04398             Vnm_tprint(2, "    Sorry; can't write z-shifted dielectric map for FEM!\n");
04399             writeit = 0;
04400             break;
04401
04402         case VDT_KAPPA:
04403
04404             Vnm_tprint(1, "    Sorry; can't write kappa map for FEM!\n");
04405             writeit = 0;
04406             break;
04407
04408         case VDT_ATOMPOT:
04409
04410             Vnm_tprint(1, "    Sorry; can't write atom potentials for FEM!\n");
04411             writeit = 0;
04412             break;
04413
04414         default:
04415
04416             Vnm_tprint(2, "Invalid data type for writing!\n");
04417             writeit = 0;
04418             return 0;
04419     }
04420
04421     if (!writeit) return 0;
04422
04423
04424     #ifdef HAVE_MPI_H
04425         sprintf(writestem, "%s-PE%d", pbeparm->writestem[i], rank);
04426     #else
04427         if(nosh->ispara){
04428             sprintf(writestem, "%s-PE%d", pbeparm->writestem[i], nosh->proc_rank);
04429         }else{
04430             sprintf(writestem, "%s", pbeparm->writestem[i]);
04431         }
04432     #endif
04433
04434     switch (pbeparm->writefmt[i]) {
04435
04436         case VDF_DX:
04437             sprintf(outpath, "%s.%s", writestem, "dx");
04438             Vnm_tprint(1, "%s\n", outpath);
04439             Vfetk_write(fetk, "FILE", "ASC", VNULL, outpath, vec, VDF_DX);
04440             break;
04441
04442         case VDF_DXBIN:
04443             //TODO: probably change some or all of below.
04444             sprintf(outpath, "%s.%s", writestem, "dxbin");
04445             Vnm_tprint(1, "%s\n", outpath);
04446             Vfetk_write(fetk, "FILE", "ASC", VNULL, outpath, vec, VDF_DXBIN);
04447             break;
04448
04449         case VDF_AVS:
04450             sprintf(outpath, "%s.%s", writestem, "ucd");
04451             Vnm_tprint(1, "%s\n", outpath);
04452             Vfetk_write(fetk, "FILE", "ASC", VNULL, outpath, vec, VDF_AVS);
04453             break;
04454
04455         case VDF_UHBD:
04456             Vnm_tprint(2, "UHBD format not supported for FEM!\n");
04457             break;
04458
04459         case VDF_MCSF:
04460             Vnm_tprint(2, "MCSF format not supported yet!\n");
04461             break;
04462
04463         default:
04464             Vnm_tprint(2, "Bogus data format (%d)!\n",

```

```

04465             pbeparm->writefmt[i]);
04466             break;
04467         }
04468     }
04469 }
04470
04471     return 1;
04472 }
04473 #endif /* ifdef HAVE_MCX_H */
04474
04475 VPUBLIC int initAPOL(Nosh *nosh,
04476                    Vmem *mem,
04477                    Vparam *param,
04478                    APOLparm *apolparm,
04479                    int *nforce,
04480                    AtomForce **atomForce,
04481                    Valist *alist
04482                ) {
04483     int i,
04484         natoms,
04485         len,
04486         inhash[3],
04487         rc = 0;
04488     time_t ts;
04489     Vclist *clist = VNULL;
04490     Vacc *acc = VNULL;
04491     Vatom *atom = VNULL;
04492     Vparam_AtomData *atomData = VNULL;
04493     double sasa,
04494            sav,
04495            nhash[3],
04496            sradPad,
04497            x,
04498            y,
04499            z,
04500            atomRadius,
04501            srad,
04502            *atomsasa,
04503            *atomwcaEnergy,
04504            energy = 0.0,
04505            dist,
04506            charge,
04507            xmin,
04508            xmax,
04509            ymin,
04510            ymax,
04511            zmin,
04512            zmax,
04513            disp[3],
04514            center[3],
04515            soluteXlen,
04516            soluteYlen,
04517            soluteZlen;
04518     atomsasa = (double *)Vmem_malloc(VNULL, Valist_getNumberAtoms(alist), sizeof(double));
04519     atomwcaEnergy = (double *)Vmem_malloc(VNULL, Valist_getNumberAtoms(alist), sizeof(double));
04520
04521     /* Determine solute length and charge*/
04522     atom = Valist_getAtom(alist, 0);
04523     xmin = Vatom_getPosition(atom)[0];
04524     xmax = Vatom_getPosition(atom)[0];
04525     ymin = Vatom_getPosition(atom)[1];
04526     ymax = Vatom_getPosition(atom)[1];
04527     zmin = Vatom_getPosition(atom)[2];
04528     zmax = Vatom_getPosition(atom)[2];
04529     charge = 0;
04530     natoms = Valist_getNumberAtoms(alist);
04531
04532     for (i=0; i < natoms; i++) {
04533         atom = Valist_getAtom(alist, i);
04534         atomRadius = Vatom_getRadius(atom);
04535         x = Vatom_getPosition(atom)[0];
04536         y = Vatom_getPosition(atom)[1];
04537         z = Vatom_getPosition(atom)[2];
04538         if ((x+atomRadius) > xmax) xmax = x + atomRadius;
04539         if ((x-atomRadius) < xmin) xmin = x - atomRadius;
04540         if ((y+atomRadius) > ymax) ymax = y + atomRadius;
04541         if ((y-atomRadius) < ymin) ymin = y - atomRadius;
04542         if ((z+atomRadius) > zmax) zmax = z + atomRadius;
04543         if ((z-atomRadius) < zmin) zmin = z - atomRadius;
04544         disp[0] = (x - center[0]);
04545         disp[1] = (y - center[1]);

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04549         disp[2] = (z - center[2]);
04550         dist = (disp[0]*disp[0]) + (disp[1]*disp[1]) + (disp[2]*disp[2]);
04551         dist = VSQRT(dist) + atomRadius;
04552         charge += Vatom_getCharge(Valist_getAtom(alist, i));
04553     }
04554     soluteXlen = xmax - xmin;
04555     soluteYlen = ymax - ymin;
04556     soluteZlen = zmax - zmin;
04557
04558     /* Set up the hash table for the cell list */
04559     Vnm_print(0, "APOL: Setting up hash table and accessibility object...\n");
04560     nhash[0] = soluteXlen/0.5;
04561     nhash[1] = soluteYlen/0.5;
04562     nhash[2] = soluteZlen/0.5;
04563     for (i=0; i<3; i++) inhash[i] = (int)(nhash[i]);
04564
04565     for (i=0; i<3; i++){
04566         if (inhash[i] < 3) inhash[i] = 3;
04567         if (inhash[i] > MAX_HASH_DIM) inhash[i] = MAX_HASH_DIM;
04568     }
04569
04570     /* Pad the radius by 2x the maximum displacement value */
04571     srاد = apolparm->srاد;
04572     srادPad = srاد + (2*apolparm->dpos);
04573     clist = Vclist_ctor(alist, srادPad, inhash, CLIST_AUTO_DOMAIN,
04574                        VNULL, VNULL);
04575     acc = Vacc_ctor(alist, clist, apolparm->sdens);
04576
04577     /* Get WAT (water) LJ parameters from Vparam object */
04578     if (param == VNULL && (apolparm->bconc != 0.0)) {
04579         Vnm_tprint(2, "initAPOL: Got NULL Vparam object!\n");
04580         Vnm_tprint(2, "initAPOL: You are performing an apolar calculation with the van der Waals integral
term,\n");
04581         Vnm_tprint(2, "initAPOL: this term requires van der Waals parameters which are not available from
the \n");
04582         Vnm_tprint(2, "initAPOL: PQR file. Therefore, you need to supply a parameter file with the parm
keyword,\n");
04583         Vnm_tprint(2, "initAPOL: for example,\n");
04584         Vnm_tprint(2, "initAPOL: read parm flat amber94.dat end\n");
04585         Vnm_tprint(2, "initAPOL: where the relevant parameter files can be found in
apbs/tools/conversion/param/vparam.\n");
04586         return VRC_FAILURE;
04587     }
04588
04589     if (apolparm->bconc != 0.0){
04590         atomData = Vparam_getAtomData(param, "WAT", "OW");
04591         if (atomData == VNULL) atomData = Vparam_getAtomData(param, "WAT", "O");
04592         if (atomData == VNULL) {
04593             Vnm_tprint(2, "initAPOL: Couldn't find parameters for WAT OW or WAT O!\n");
04594             Vnm_tprint(2, "initAPOL: These parameters must be present in your file\n");
04595             Vnm_tprint(2, "initAPOL: for apolar calculations.\n");
04596             return VRC_FAILURE;
04597         }
04598         apolparm->watepsilon = atomData->epsilon;
04599         apolparm->watsigma = atomData->radius;
04600         apolparm->setwat = 1;
04601     }
04602
04603     /* Calculate Energy and Forces */
04604     if (apolparm->calcforce) {
04605         rc = forceAPOL(acc, mem, apolparm, nforce, atomForce, alist, clist);
04606         if (rc == VRC_FAILURE) {
04607             Vnm_print(2, "Error in apolar force calculation!\n");
04608             return VRC_FAILURE;
04609         }
04610     }
04611
04612     /* Get the SAV and SAS */
04613     sasa = 0.0;
04614     sav = 0.0;
04615
04616     if (apolparm->calcenergy) {
04617         len = Valist_getNumberAtoms(alist);
04618
04619         if (VABS(apolparm->gamma) > VSMALL) {
04620             /* Total Solvent Accessible Surface Area (SASA) */
04621             apolparm->sasa = Vacc_totalSASA(acc, srاد);
04622             /* SASA for each atom */
04623             for (i = 0; i < len; i++) {
04624                 atom = Valist_getAtom(alist, i);
04625                 atomsasa[i] = Vacc_atomSASA(acc, srاد, atom);

```

```

04626     }
04627   } else {
04628     /* Total Solvent Accessible Surface Area (SASA) set to zero */
04629     apolparm->sasa = 0.0;
04630     /* SASA for each atom set to zero*/
04631     for (i = 0; i < len; i++) {
04632       atomsasa[i] = 0.0;
04633     }
04634   }
04635
04636   /* Inflated van der Waals accessibility */
04637   if (VABS(apolparm->press) > VSMALL) {
04638     apolparm->sav = Vacci_totalSAV(acc, clist, apolparm, srاد);
04639   } else {
04640     apolparm->sav = 0.0;
04641   }
04642
04643   /* wcaEnergy integral code */
04644   if (VABS(apolparm->bconc) > VSMALL) {
04645     /* wcaEnergy for each atom */
04646     for (i = 0; i < len; i++) {
04647       rc = Vacci_wcaEnergyAtom(acc, apolparm, alist, clist, i, &energy);
04648       if (rc == 0) {
04649         Vnm_print(2, "Error in apolar energy calculation!\n");
04650         return 0;
04651       }
04652       atomwcaEnergy[i] = energy;
04653     }
04654     /* Total WCA Energy */
04655     rc = Vacci_wcaEnergy(acc, apolparm, alist, clist);
04656     if (rc == 0) {
04657       Vnm_print(2, "Error in apolar energy calculation!\n");
04658       return 0;
04659     }
04660   } else {
04661     apolparm->wcaEnergy = 0.0;
04662   }
04663   energyAPOL(apolparm, apolparm->sasa, apolparm->sav, atomsasa, atomwcaEnergy,
Valist_getNumberAtoms(alist));
04664 }
04665
04666 Vmem_free(VNULL, Valist_getNumberAtoms(alist), sizeof(double), (void *)&(atomsasa));
04667 Vmem_free(VNULL, Valist_getNumberAtoms(alist), sizeof(double), (void *)&(atomwcaEnergy));
04668 Vclist_dtor(&clist);
04669 Vacci_dtor(&acc);
04670
04671 return VRC_SUCCESS;
04672 }
04673
04674 VPUBLIC int energyAPOL(APOLparm *apolparm,
double sasa,
double sav,
double atomsasa[],
double atomwcaEnergy[],
int numatoms
){
04680
04681
04682 double energy = 0.0;
04683 int i = 0;
04684
04685 #ifndef VAPBSQUIET
04686 Vnm_print(1, "\nSolvent Accessible Surface Area (SASA) for each atom:\n");
04687 for (i = 0; i < numatoms; i++) {
04688   Vnm_print(1, " SASA for atom %i: %1.12E\n", i, atomsasa[i]);
04689 }
04690
04691 Vnm_print(1, "\nTotal solvent accessible surface area: %g A^2\n", sasa);
04692 #endif
04693
04694 switch(apolparm->calcenergy) {
04695   case ACE_NO:
04696     break;
04697   case ACE_COMPS:
04698     Vnm_print(1, "energyAPOL: Cannot calculate component energy, skipping.\n");
04699     break;
04700   case ACE_TOTAL:
04701     energy = (apolparm->gamma*sasa) + (apolparm->press*sav)
+ (apolparm->wcaEnergy);
04702
04703 #ifndef VAPBSQUIET
04704 Vnm_print(1, "\nSurface tension*area energies (gamma * SASA) for each atom:\n");
04705 for (i = 0; i < numatoms; i++) {

```

```

04706         Vnm_print(1, " Surface tension*area energy for atom %i: %1.12E\n", i,
apolparm->gamma*atomsasa[i]);
04707     }
04708
04709     Vnm_print(1, "\nTotal surface tension energy: %g kJ/mol\n", apolparm->gamma*sasa);
04710     Vnm_print(1, "\nTotal solvent accessible volume: %g A^3\n", sav);
04711     Vnm_print(1, "\nTotal pressure*volume energy: %g kJ/mol\n", apolparm->press*sav);
04712     Vnm_print(1, "\nWCA dispersion Energies for each atom:\n");
04713     for (i = 0; i < numatoms; i++) {
04714         Vnm_print(1, " WCA energy for atom %i: %1.12E\n", i, atomwcaEnergy[i]);
04715     }
04716
04717     Vnm_print(1, "\nTotal WCA energy: %g kJ/mol\n", (apolparm->wcaEnergy));
04718     Vnm_print(1, "\nTotal non-polar energy = %1.12E kJ/mol\n", energy);
04719 #endif
04720     break;
04721     default:
04722         Vnm_print(2, "energyAPOL: Error in energyAPOL. Unknown option.\n");
04723         break;
04724     }
04725
04726     return VRC_SUCCESS;
04727 }
04728
04729 VPUBLIC int forceAPOL(Vacc *acc,
04730                     Vmem *mem,
04731                     APOLparm *apolparm,
04732                     int *nforce,
04733                     AtomForce **atomForce,
04734                     Valist *alist,
04735                     Vclist *clist
04736                     ) {
04737     time_t ts, ts_main, ts_sub;
04738
04739     int i,
04740         j,
04741         natom;
04742
04743     double srad, /* Probe radius */
04744         xF,
04745         yF,
04746         zF, /* Individual forces */
04747         press,
04748         gamma,
04749         offset,
04750         bconc,
04751         dSASA[3],
04752         dSAV[3],
04753         force[3],
04754         *apos;
04755
04756     Vatom *atom = VNULL;
04757     ts_main = clock();
04758
04759     srad = apolparm->srad;
04760     press = apolparm->press;
04761     gamma = apolparm->gamma;
04762     offset = apolparm->dpos;
04763     bconc = apolparm->bconc;
04764
04765     natom = Valist_getNumberAtoms(alist);
04766
04767     /* Check to see if we need to build the surface */
04768     Vnm_print(0, "forceAPOL: Trying atom surf...\n");
04769     ts = clock();
04770     if (acc->surf == VNULL) {
04771         acc->surf = (VaccSurf**)Vmem_malloc(acc->mem, natom, sizeof(VaccSurf *));
04772         for (i=0; i<natom; i++) {
04773             atom = Valist_getAtom(acc->alist, i);
04774             //apos = Vatom_getPosition(atom); // apos never referenced? - Peter
04775             /* NOTE: RIGHT NOW WE DO THIS FOR THE ENTIRE MOLECULE WHICH IS
04776              * INCREDIBLY INEFFICIENT, PARTICULARLY DURING FOCUSING!!! */
04777             acc->surf[i] = Vacc_atomSurf(acc, atom, acc->refSphere, srad);
04778         }
04779     }
04780     Vnm_print(0, "forceAPOL: atom surf: Time elapsed: %f\n", ((double)clock() - ts) / CLOCKS_PER_SEC);
04781
04782     if (apolparm->calcforce == ACF_TOTAL) {
04783         Vnm_print(0, "forceAPOL: calcforce == ACF_TOTAL\n");
04784         ts = clock();
04785
04786         *nforce = 1;

```



```

04786     if(*atomForce != VNULL){
04787         Vmem_free(mem,*nforce,sizeof(AtomForce), (void **)atomForce);
04788     }
04789
04790     *atomForce = (AtomForce *)Vmem_malloc(mem, *nforce,
04791                                           sizeof(AtomForce));
04792
04793     /* Clear out force arrays */
04794     for (j=0; j<3; j++) {
04795         (*atomForce)[0].sasaForce[j] = 0.0;
04796         (*atomForce)[0].savForce[j] = 0.0;
04797         (*atomForce)[0].wcaForce[j] = 0.0;
04798     }
04799
04800     // problem block
04801     for (i=0; i<natom; i++) {
04802         atom = Valist_getAtom(alist, i);
04803
04804         for(j=0;j<3;j++){
04805             dSASA[j] = 0.0;
04806             dSAV[j] = 0.0;
04807             force[j] = 0.0;
04808         }
04809
04810         if(VABS(gamma) > VSMALL) {
04811             Vacc_atomdSASA(acc, offset, srاد, atom, dSASA);
04812         }
04813         if(VABS(press) > VSMALL) {
04814             Vacc_atomdSAV(acc, srاد, atom, dSAV);
04815         }
04816         if(VABS(bconc) > VSMALL) {
04817             Vacc_wcaForceAtom(acc, apolparm, clist, atom, force);
04818         }
04819
04820         for(j=0;j<3;j++){
04821             (*atomForce)[0].sasaForce[j] += dSASA[j];
04822             (*atomForce)[0].savForce[j] += dSAV[j];
04823             (*atomForce)[0].wcaForce[j] += force[j];
04824         }
04825     }
04826     // end block
04827
04828     Vnm_tprint( 1, " Printing net forces (kJ/mol/A)\n");
04829     Vnm_tprint( 1, " Legend:\n");
04830     Vnm_tprint( 1, "      sasa -- SASA force\n");
04831     Vnm_tprint( 1, "      sav  -- SAV force\n");
04832     Vnm_tprint( 1, "      wca  -- WCA force\n\n");
04833
04834     Vnm_tprint( 1, " sasa %4.3e %4.3e %4.3e\n",
04835               (*atomForce)[0].sasaForce[0],
04836               (*atomForce)[0].sasaForce[1],
04837               (*atomForce)[0].sasaForce[2]);
04838     Vnm_tprint( 1, " sav   %4.3e %4.3e %4.3e\n",
04839               (*atomForce)[0].savForce[0],
04840               (*atomForce)[0].savForce[1],
04841               (*atomForce)[0].savForce[2]);
04842     Vnm_tprint( 1, " wca   %4.3e %4.3e %4.3e\n",
04843               (*atomForce)[0].wcaForce[0],
04844               (*atomForce)[0].wcaForce[1],
04845               (*atomForce)[0].wcaForce[2]);
04846
04847     Vnm_print(0, "forceAPOL: calcforce == ACF_TOTAL: %f\n", ((double)clock() - ts) / CLOCKS_PER_SEC);
04848 } else if (apolparm->calcforce == ACF_COMPS ){
04849     *nforce = Valist_getNumberAtoms(alist);
04850     if(*atomForce == VNULL){
04851         *atomForce = (AtomForce *)Vmem_malloc(mem, *nforce,
04852                                               sizeof(AtomForce));
04853     }else{
04854         Vmem_free(mem,*nforce,sizeof(AtomForce), (void **)atomForce);
04855         *atomForce = (AtomForce *)Vmem_malloc(mem, *nforce,
04856                                               sizeof(AtomForce));
04857     }
04858
04859 #ifndef VAPBSQUIET
04860     Vnm_tprint( 1, " Printing per atom forces (kJ/mol/A)\n");
04861     Vnm_tprint( 1, " Legend:\n");
04862     Vnm_tprint( 1, "      tot n -- Total force for atom n\n");
04863     Vnm_tprint( 1, "      sasa n -- SASA force for atom n\n");
04864     Vnm_tprint( 1, "      sav  n -- SAV force for atom n\n");
04865     Vnm_tprint( 1, "      wca  n -- WCA force for atom n\n\n");
04866

```

```

04867         Vnm_tprint( 1, "      gamma      %f\n" \
04868                      "      pressure %f\n" \
04869                      "      bconc      %f\n\n",
04870                      gamma,press,bconc);
04871 #endif
04872
04873     for (i=0; i<natom; i++) {
04874         atom = Valist_getAtom(alist, i);
04875
04876         for (j=0; j<3; j++) {
04877             dSASA[j] = 0.0;
04878             dSAV[j] = 0.0;
04879             force[j] = 0.0;
04880         }
04881
04882         /* Clear out force arrays */
04883         for (j=0; j<3; j++) {
04884             (*atomForce)[i].sasaForce[j] = 0.0;
04885             (*atomForce)[i].savForce[j] = 0.0;
04886             (*atomForce)[i].wcaForce[j] = 0.0;
04887         }
04888
04889         if (VABS(gamma) > VSMALL) Vacci_atomdSASA(acc, offset, srاد, atom, dSASA);
04890         if (VABS(press) > VSMALL) Vacci_atomdSAV(acc, srاد, atom, dSAV);
04891         if (VABS(bconc) > VSMALL) Vacci_wcaForceAtom(acc,apolparm,clist,atom,force);
04892
04893         xF = -((gamma*dSASA[0]) + (press*dSAV[0]) + (bconc*force[0]));
04894         yF = -((gamma*dSASA[1]) + (press*dSAV[1]) + (bconc*force[1]));
04895         zF = -((gamma*dSASA[2]) + (press*dSAV[2]) + (bconc*force[2]));
04896
04897         for (j=0; j<3; j++) {
04898             (*atomForce)[i].sasaForce[j] += dSASA[j];
04899             (*atomForce)[i].savForce[j] += dSAV[j];
04900             (*atomForce)[i].wcaForce[j] += force[j];
04901         }
04902
04903 #ifndef VAPBSQUIET
04904         Vnm_print( 1, "    tot  %i %4.3e %4.3e %4.3e\n",
04905                  i,
04906                  xF,
04907                  yF,
04908                  zF);
04909         Vnm_print( 1, "    sasa %i %4.3e %4.3e %4.3e\n",
04910                  i,
04911                  (*atomForce)[i].sasaForce[0],
04912                  (*atomForce)[i].sasaForce[1],
04913                  (*atomForce)[i].sasaForce[2]);
04914         Vnm_print( 1, "    sav  %i %4.3e %4.3e %4.3e\n",
04915                  i,
04916                  (*atomForce)[i].savForce[0],
04917                  (*atomForce)[i].savForce[1],
04918                  (*atomForce)[i].savForce[2]);
04919         Vnm_print( 1, "    wca  %i %4.3e %4.3e %4.3e\n",
04920                  i,
04921                  (*atomForce)[i].wcaForce[0],
04922                  (*atomForce)[i].wcaForce[1],
04923                  (*atomForce)[i].wcaForce[2]);
04924 #endif
04925     }
04926 } else *nforce = 0;
04927
04928 #ifndef VAPBSQUIET
04929     Vnm_print(1,"\\n");
04930 #endif
04931
04932     Vnm_print(0, "forceAPOL: Time elapsed: %f\\n", ((double)clock() - ts_main) / CLOCKS_PER_SEC);
04933     return VRC_SUCCESS;
04934 }
04935
04936
04937 #ifdef ENABLE_BEM
04938 VPUBLIC int initBEM(int icalc,
04939                   NOsh *nosh,
04940                   BEMparm *bemparm,
04941                   PBEparm *pbeparm,
04942                   Vpbe *pbe[NOSH_MAXCALC]
04943                   ) {
04944
04945     Vnm_tstart(APBS_TIMER_SETUP, "Setup timer");
04946
04947
04948
04949
04950

```

```
04951      /* Setup time statistics */
04952      Vnm_tstop(APBS_TIMER_SETUP, "Setup timer");
04953
04954      return 1;
04955
04956 }
04957
04958 VPUBLIC void killBEM(Nosh *nosh, Vpbe *pbe[NOSH_MAXCALC]
04959                    ) {
04960
04961     int i;
04962
04963 #ifndef VAPBSQUIET
04964     Vnm_tprint(1, "Destroying boundary element structures.\n");
04965 #endif
04966
04967 }
04968
04969
04970
04971 void apbs2tabipb_(TABIPBparm* tabiparm,
04972                  TABIPBvars* tabivars);
04973
04974 VPUBLIC int solveBEM(Valist* molecules[NOSH_MAXMOL],
04975                    Nosh *nosh,
04976                    PBEparm *pbeparm,
04977                    BEMparm *bemparm,
04978                    BEMparm_CalcType type) {
04979
04980     int nx,
04981         ny,
04982         nz,
04983         i;
04984
04985     if (nosh != VNULL) {
04986         if (nosh->bogus) return 1;
04987     }
04988
04989     Vnm_tstart(APBS_TIMER_SOLVER, "Solver timer");
04990
04991     TABIPBparm *tabiparm = (TABIPBparm*)calloc(1, sizeof(TABIPBparm));
04992
04993     sprintf(tabiparm->fpath, "");
04994     strncpy(tabiparm->fname, nosh->molpath[0], 4);
04995     tabiparm->fname[4] = '\0';
04996     tabiparm->density = pbeparm->sdens;
04997     tabiparm->probe_radius = pbeparm->srad;
04998
04999     tabiparm->eps = pbeparm->pdie;
05000     tabiparm->epsw = pbeparm->sdie;
05001     tabiparm->bulk_strength = 0.0;
05002     for (i=0; i<pbeparm->nion; i++)
05003         tabiparm->bulk_strength += pbeparm->ionc[i]
05004                                   *pbeparm->ionq[i]*pbeparm->ionq[i];
05005     tabiparm->temp = pbeparm->temp;
05006
05007     tabiparm->order = bemparm->tree_order;
05008     tabiparm->maxparnode = bemparm->tree_n0;
05009     tabiparm->theta = bemparm->mac;
05010
05011     tabiparm->mesh_flag = bemparm->mesh;
05012
05013     tabiparm->number_of_lines = Valist_getNumberAtoms(molecules[0]);
05014
05015     tabiparm->output_datafile = bemparm->outdata;
05016
05017     TABIPBvars *tabivars = (TABIPBvars*)calloc(1, sizeof(TABIPBvars));
05018     if ((tabivars->chrpos = (double *) malloc(3 * tabiparm->number_of_lines * sizeof(double))) == NULL) {
05019         printf("Error in allocating t_chrpos!\n");
05020     }
05021     if ((tabivars->atmchr = (double *) malloc(tabiparm->number_of_lines * sizeof(double))) == NULL) {
05022         printf("Error in allocating t_atmchr!\n");
05023     }
05024     if ((tabivars->atmrad = (double *) malloc(tabiparm->number_of_lines * sizeof(double))) == NULL) {
05025         printf("Error in allocating t_atmrad!\n");
05026     }
05027
05028     Vatom *atom;
05029
05030     for (i = 0; i < tabiparm->number_of_lines; i++){
05031         atom = Valist_getAtom(molecules[0], i);
```

```

05032     tabivars->chrpos[3*i] = Vatom_getPosition(atom)[0];
05033     tabivars->chrpos[3*i + 1] = Vatom_getPosition(atom)[1];
05034     tabivars->chrpos[3*i + 2] = Vatom_getPosition(atom)[2];
05035     tabivars->atmchr[i] = Vatom_getCharge(atom);
05036     tabivars->atmrad[i] = Vatom_getRadius(atom);
05037 }
05038
05039 //apbs2tabipb(TABIPBparm* tabiparm, Valist* molecules[NOSH_MAXMOL]);
05040 apbs2tabipb(tabiparm, tabivars);
05041
05042 free(tabiparm);
05043 free(tabivars->chrpos);
05044 free(tabivars->atmchr);
05045 free(tabivars->atmrad);
05046 free(tabivars->vert_ptl); // allocate in output_potential()
05047 free(tabivars->xvct); // allocate in output_potential()
05048 free_matrix(tabivars->vert); // allocate in output_potential()
05049 free_matrix(tabivars->snrm); // allocate in output_potential()
05050 free_matrix(tabivars->face); // allocate in output_potential()
05051
05052 Vnm_tprint(1, "\n\nReturning to APBS caller...\n\n");
05053 Vnm_tprint(1, "Solvation energy and Coulombic energy in kJ/mol...\n\n");
05054 Vnm_tprint(1, "  Global net ELEC energy = %1.12E\n", tabivars->soleng);
05055 Vnm_tprint(1, "  Global net COULOMBIC energy = %1.12E\n\n", tabivars->couleng);
05056
05057 free(tabivars);
05058
05059 Vnm_tstop(APBS_TIMER_SOLVER, "Solver timer");
05060
05061 return 1;
05062 }
05063 }
05064
05065 VPUBLIC int setPartBEM(NOsh *nosh,
05066                      BEMparm *BEMparm
05067                      ) {
05068
05069     int j;
05070     double partMin[3],
05071            partMax[3];
05072
05073     if (nosh->bogus) return 1;
05074
05075     return 1;
05076
05077 }
05078
05079 VPUBLIC int energyBEM(NOsh *nosh,
05080                     int icalc,
05081                     int *nenergy,
05082                     double *totEnergy,
05083                     double *qfEnergy,
05084                     double *qmEnergy,
05085                     double *dielEnergy
05086                     ) {
05087
05088     Valist *alist;
05089     Vatom *atom;
05090     int i,
05091          extEnergy;
05092     double tenergy;
05093     BEMparm *bemparm;
05094     PBEParm *pbeparm;
05095
05096     bemparm = nosh->calc[icalc]->bemparm;
05097     pbeparm = nosh->calc[icalc]->pbeparm;
05098
05099     Vnm_tstart(APBS_TIMER_ENERGY, "Energy timer");
05100     Vnm_tstop(APBS_TIMER_ENERGY, "Energy timer");
05101
05102     return 1;
05103 }
05104
05105 VPUBLIC int forceBEM(
05106     NOsh *nosh,
05107     PBEParm *pbeparm,
05108     BEMparm *bemparm,
05109     int *nforce,
05110     AtomForce **atomForce,
05111     Valist *alist[NOSH_MAXMOL]
05112 ) {

```

```
05113
05114     int j,
05115         k;
05116     double qfForce[3],
05117         dbForce[3],
05118         ibForce[3];
05119
05120     Vnm_tstart(APBS_TIMER_FORCE, "Force timer");
05121
05122 #ifndef VAPBSQUIET
05123     Vnm_tprint( 1, " Calculating forces...\n");
05124 #endif
05125
05126     Vnm_tstop(APBS_TIMER_FORCE, "Force timer");
05127
05128     return 1;
05129 }
05130
05131 VPUBLIC void printBEMPARM(BEMParm *bemparm) {
05132
05133 }
05134
05135
05136 VPUBLIC int writedataBEM(int rank,
05137                         NOsh *nosh,
05138                         PBEparm *pbeparm
05139                     ) {
05140
05141     return 1;
05142 }
05143
05144
05145 VPUBLIC int writematBEM(int rank, NOsh *nosh, PBEparm *pbeparm) {
05146
05147     if (nosh->bogus) return 1;
05148     return 1;
05149 }
05150
05151 #endif
05152
05153
05154 #ifdef ENABLE_GEOFLOW
05155
05156 VPUBLIC int solveGeometricFlow( Valist* molecules[NOSH_MAXMOL],
05157                               NOsh *nosh,
05158                               PBEparm *pbeparm,
05159                               APOLparm *apolparm,
05160                               GEOFLOWparm *parm )
05161 {
05162     //printf("solveGeometricFlow!!!\n");
05163     if (nosh != VNULL) {
05164         if (nosh->bogus) return 1;
05165     }
05166
05167     Vnm_tstart(APBS_TIMER_SOLVER, "Solver timer");
05168
05169     struct GeometricFlowInput geoflowIn = getGeometricFlowParams();
05170
05171     // change any of the parameters you want...
05172     geoflowIn.m_boundaryCondition = (int) pbeparm->bcfl ;
05173     geoflowIn.m_grid[0] = apolparm->grid[0];
05174     geoflowIn.m_grid[1] = apolparm->grid[1];
05175     geoflowIn.m_grid[2] = apolparm->grid[2];
05176     geoflowIn.m_gamma = apolparm->gamma;
05177     geoflowIn.m_pdie = pbeparm->pdie ;
05178     geoflowIn.m_sdie = pbeparm->sdie ;
05179     geoflowIn.m_press = apolparm->press ;
05180     geoflowIn.m_tol = parm->etol;
05181     geoflowIn.m_bconc = apolparm->bconc ;
05182     geoflowIn.m_vdwdispersion = parm->vdw;
05183     geoflowIn.m_etolSolvation = .01 ; // to be added?
05184
05185     // debug
05186     //printGeometricFlowStruct( geoflowIn );
05187
05188     //printf("num mols: %i\n", nosh->nmol);
05189     struct GeometricFlowOutput geoflowOut =
05190         runGeometricFlowWrapAPBS( geoflowIn, molecules[0] );
05191
05192     Vnm_tprint( 1, " Global net energy = %1.12E\n", geoflowOut.m_totalSolvation);
```

```

05197     Vnm_tprint( 1,"   Global net ELEC energy = %1.12E\n", geoflowOut.m_elecSolvation);
05198     Vnm_tprint( 1,"   Global net APOL energy = %1.12E\n", geoflowOut.m_nonpolarSolvation);
05199
05200     Vnm_tstop(APBS_TIMER_SOLVER, "Solver timer");
05201
05202     return 1;
05203 }
05204 }
05205
05206 #endif
05207
05208 #ifdef ENABLE_PBAM
05209
05210 VPUBLIC int solvePBAM( Valist* molecules[NOSH_MAXMOL],
05211                     NOSH *nosh,
05212                     PBEparam *pbeparm,
05213                     PBAMparam *param )
05214 {
05215     if (nosh != VNULL) {
05216         if (nosh->bogus) return 1;
05217     }
05218
05219     int i, j;
05220     Vnm_tstart(APBS_TIMER_SOLVER, "Solver timer");
05221     PBAMInput pbamIn = getPBAMParams();
05222
05223     pbamIn.nmol_ = nosh->nmol;
05224
05225     // change any of the parameters you want...
05226     pbamIn.temp_ = pbeparm->temp;
05227     if (fabs(pbamIn.temp_-0.0) < 1e-3)
05228     {
05229         printf("No temperature specified. Setting to 298.15K\n");
05230         pbamIn.temp_ = 298.15;
05231     }
05232
05233     // Dielectrics
05234     pbamIn.idiel_ = pbeparm->pdie;
05235     pbamIn.sdiel_ = pbeparm->sdiel;
05236
05237     // Salt conc
05238     pbamIn.salt_ = param->salt;
05239
05240     // Runtime: can be energyforce, electrostatics etc
05241     strncpy(pbamIn.runType_, param->runtype, CHR_MAXLEN);
05242     strncpy(pbamIn.runName_, param->runname, CHR_MAXLEN);
05243
05244     pbamIn.randOrient_ = param->setrandorient;
05245
05246     pbamIn.boxLen_ = param->pbcbboxlen;
05247     pbamIn.pbcType_ = param->setpbc;
05248
05249     pbamIn.setunits_ = param->setunits;
05250     if(param->setunits == 1) strncpy(pbamIn.units_, param->units, CHR_MAXLEN);
05251
05252     // Electrostatic stuff
05253     if (param->setgridpt) pbamIn.gridPts_ = param->gridpt;
05254     strncpy(pbamIn.map3D_, param->map3dname, CHR_MAXLEN);
05255     pbamIn.grid2Dct_ = param->grid2Dct;
05256     for (i=0; i<pbamIn.grid2Dct; i++)
05257     {
05258         strncpy(pbamIn.grid2D_[i], param->grid2Dname[i], CHR_MAXLEN);
05259         strncpy(pbamIn.grid2Dax_[i], param->grid2Dax[i], CHR_MAXLEN);
05260         pbamIn.grid2Dloc_[i] = param->grid2Dloc[i];
05261     }
05262     strncpy(pbamIn.dxname_, param->dxname, CHR_MAXLEN);
05263
05264     // Dynamics stuff
05265     pbamIn.ntraj_ = param->ntraj;
05266     strncpy(pbamIn.termCombine_, param->termcombine, CHR_MAXLEN);
05267
05268     pbamIn.termct_ = param->termct;
05269     pbamIn.contct_ = param->confilct;
05270
05271     if (strcmp(pbamIn.runType_, "dynamics", 8) == 0)
05272     {
05273         if (pbamIn.nmol_ > param->diffct)
05274         {
05275             Vnm_tprint(2, "You need more diffusion information!\n");
05276             return 0;
05277         }
05278     }
05279 }
05280

```

```
05281
05282     for (i=0; i<pbamIn.nmol_; i++)
05283     {
05284         if (parm->xyzct[i] < parm->ntraj)
05285         {
05286             Vnm_tprint(2, "For molecule %d, you are missing trajectory!\n", i+1);
05287             return 0;
05288         } else {
05289             for (j=0; j<pbamIn.ntraj_; j++)
05290             {
05291                 strncpy(pbamIn.xyzfil_[i][j], parm->xyzfil[i][j], CHR_MAXLEN);
05292             }
05293         }
05294     }
05295
05296     for (i=0; i<pbamIn.nmol_; i++)
05297     {
05298         strncpy(pbamIn.moveType_[i], parm->moveType[i], CHR_MAXLEN);
05299         pbamIn.transDiff_[i] = parm->transDiff[i];
05300         pbamIn.rotDiff_[i] = parm->rotDiff[i];
05301     }
05302
05303     for (i=0; i<pbamIn.termct_; i++)
05304     {
05305         strncpy(pbamIn.termnam_[i], parm->termnam[i], CHR_MAXLEN);
05306         pbamIn.termnu_[i][0] = parm->termnu[i][0];
05307         pbamIn.termval_[i] = parm->termVal[i];
05308     }
05309
05310     for (i=0; i<pbamIn.contct_; i++)
05311     {
05312         strncpy(pbamIn.confil_[i], parm->confil[i], CHR_MAXLEN);
05313     }
05314 }
05315
05316 // debug
05317 printPBAMStruct( pbamIn );
05318
05319 // Run the darn thing
05320 PBAMOutput pbamOut = runPBAMWrapAPBS( pbamIn, molecules, nosh->nmol );
05321
05322 Vnm_tprint(1, "\n\nReturning to APBS caller...\n\n");
05323
05324 if (!(strcmp(pbamIn.runType_, "dynamics", 8) &&
05325         strcmp(pbamIn.runType_, "energyforce", 11))) {
05326
05327     if (!(strcmp(pbamIn.units_, "kcalmol", 7))) { //scale to kjmol is 4.18400
05328
05329         Vnm_tprint(1, "Interaction energy in kCal/mol...\n\n");
05330
05331         for (int i = 0; i < PBAMPARM_MAXMOL; i++) {
05332             Vnm_tprint(1, "  Molecule %d: Global net ELEC energy = %1.12E\n",
05333                 i+1, pbamOut.energies_[i]);
05334             Vnm_tprint(1, "          Force = (%1.6E, %1.6E, %1.6E)\n\n",
05335                 pbamOut.forces_[i][0], pbamOut.forces_[i][1],
05336                 pbamOut.forces_[i][2]);
05337             if (pbamOut.energies_[i+1] == 0.) break;
05338         }
05339     } else if (!(strcmp(pbamIn.units_, "jmol", 4))) { //scale to kjmol is 0.001
05340
05341         Vnm_tprint(1, "Interaction energy in J/mol...\n\n");
05342
05343         for (int i = 0; i < PBAMPARM_MAXMOL; i++) {
05344             Vnm_tprint(1, "  Molecule %d: Global net ELEC energy = %1.12E\n",
05345                 i+1, pbamOut.energies_[i]);
05346             Vnm_tprint(1, "          Force = (%1.6E, %1.6E, %1.6E)\n\n",
05347                 pbamOut.forces_[i][0], pbamOut.forces_[i][1],
05348                 pbamOut.forces_[i][2]);
05349             if (pbamOut.energies_[i+1] == 0.) break;
05350         }
05351     } else { // if (!(strcmp(pbamIn.units_, "kT", 2))) //scale to kjmol is 2.478 @ 298K
05352         // or 0.008315436242 * 298
05353
05354         Vnm_tprint(1, "Interaction energy in kT @ %6.2f K...\n\n", pbamIn.temp_);
05355
05356         for (int i = 0; i < PBAMPARM_MAXMOL; i++) {
05357             Vnm_tprint(1, "  Molecule %d: Global net ELEC energy = %1.12E\n",
05358                 i+1, pbamOut.energies_[i]);
05359         }
05360     }
05361 }
```

```

05362             Vnm_tprint(1, "                Force = (%1.6E, %1.6E, %1.6E)\n\n",
05363                     pbamOut.forces_[i][0], pbamOut.forces_[i][1],
05364                     pbamOut.forces_[i][2]);
05365             if (pbamOut.energies_[i+1] == 0.) break;
05366         }
05367     }
05368 }
05369 Vnm_tstop(APBS_TIMER_SOLVER, "Solver timer");
05370
05371 return 1;
05372 }
05373 }
05374 #endif
05375
05376 #ifdef ENABLE_PBSAM
05377 #define solvePBSAM( Valist* molecules[NOSH_MAXMOL],
05378                 NOSH *nosh,
05379                 PBEparam *pbeparm,
05380                 PBAMparam *parm,
05381                 PBSAMparam *sampparm )
05382 {
05383     printf("solvePBSAM!!!\n");
05384     char fname_tp[VMAX_ARGLEN];
05385     if (nosh != VNULL) {
05386         if (nosh->bogus) return 1;
05387     }
05388
05389     int i, j, k, ierr;
05390     Vnm_tstart(APBS_TIMER_SOLVER, "Solver timer");
05391     PBSAMInput pbsamIn = getPBSAMParams();
05392     PBAMInput pbamIn; // = getPBAMParams();
05393
05394     pbamIn.nmol_ = nosh->nmol;
05395
05396     // change any of the parameters you want...
05397     pbamIn.temp_ = pbeparm->temp;
05398     if (fabs(pbamIn.temp_-0.0) < 1e-3)
05399     {
05400         printf("No temperature specified. Setting to 298.15K\n");
05401         pbamIn.temp_ = 298.15;
05402     }
05403
05404     // Dielectrics
05405     pbamIn.idiel_ = pbeparm->pdie;
05406     pbamIn.sdiel_ = pbeparm->sdiel;
05407
05408     // Salt conc
05409     pbamIn.salt_ = parm->salt;
05410
05411     // Runtype: can be energyforce, electrostatics etc
05412     strncpy(pbamIn.runType_, parm->runtype, CHR_MAXLEN);
05413     strncpy(pbamIn.runName_, parm->runname, CHR_MAXLEN);
05414
05415     pbamIn.setunits_ = parm->setunits;
05416     if (parm->setunits == 1) strncpy(pbamIn.units_, parm->units, CHR_MAXLEN);
05417     pbamIn.randOrient_ = parm->setrandorient;
05418
05419     pbamIn.boxLen_ = parm->pbcbboxlen;
05420     pbamIn.pbcType_ = parm->setpbc;
05421
05422     // Electrostatic stuff
05423     if (parm->setgridpt) pbamIn.gridPts_ = parm->gridpt;
05424     strncpy(pbamIn.map3D_, parm->map3dname, CHR_MAXLEN);
05425     pbamIn.grid2Dct_ = parm->grid2Dct;
05426     for (i=0; i<pbamIn.grid2Dct_; i++)
05427     {
05428         strncpy(pbamIn.grid2D_[i], parm->grid2Dname[i], CHR_MAXLEN);
05429         strncpy(pbamIn.grid2Dax_[i], parm->grid2Dax[i], CHR_MAXLEN);
05430         pbamIn.grid2Dloc_[i] = parm->grid2Dloc[i];
05431     }
05432     strncpy(pbamIn.dxname_, parm->dxname, CHR_MAXLEN);
05433
05434     // Dynamics stuff
05435     pbamIn.ntraj_ = parm->ntraj;
05436     strncpy(pbamIn.termCombine_, parm->termcombine, CHR_MAXLEN);
05437
05438     pbamIn.termct_ = parm->termct;
05439     pbamIn.contct_ = parm->confilct;
05440 }
05441 #endif
05442

```



```

05446 if (strcmp(pbamIn.runType_, "dynamics", 8)== 0)
05447 {
05448     if (pbamIn.nmol_ > parm->diffct)
05449     {
05450         Vnm_tprint(2, "You need more diffusion information!\n");
05451         return 0;
05452     }
05453
05454     for (i=0; i<pbamIn.nmol_; i++)
05455     {
05456         if (parm->xyzct[i] < parm->ntraj)
05457         {
05458             Vnm_tprint(2, "For molecule %d, you are missing trajectory!\n", i+1);
05459             return 0;
05460         } else {
05461             for (j=0; j<pbamIn.ntraj_; j++)
05462             {
05463                 strncpy(pbamIn.xyzfil_[i][j], parm->xyzfil[i][j], CHR_MAXLEN);
05464             }
05465         }
05466     }
05467
05468     for (i=0; i<pbamIn.nmol_; i++)
05469     {
05470         strncpy(pbamIn.moveType_[i], parm->moveType[i], CHR_MAXLEN);
05471         pbamIn.transDiff_[i] = parm->transDiff[i];
05472         pbamIn.rotDiff_[i] = parm->rotDiff[i];
05473     }
05474
05475     for (i=0; i<pbamIn.termct_; i++)
05476     {
05477         strncpy(pbamIn.termnam_[i], parm->termnam[i], CHR_MAXLEN);
05478         pbamIn.termnu_[i][0] = parm->termnu[i][0];
05479         pbamIn.termval_[i] = parm->termVal[i];
05480     }
05481
05482     for (i=0; i<pbamIn.contct_; i++)
05483     {
05484         strncpy(pbamIn.confil_[i], parm->confil[i], CHR_MAXLEN);
05485     }
05486 }
05487
05488 // SAM details
05489 pbsamIn.tolsp_ = samparm->tolsp;
05490 pbsamIn.imatct_ = samparm->imatct;
05491 pbsamIn.expct_ = samparm->expct;
05492 for (i=0; i<samparm->surfct; i++)
05493 {
05494     strncpy(pbsamIn.surf[fil_][i], samparm->surf[fil][i], CHR_MAXLEN);
05495 }
05496
05497 for (i=0; i<samparm->imatct; i++)
05498 {
05499     strncpy(pbsamIn.imat[fil_][i], samparm->imat[fil][i], CHR_MAXLEN);
05500 }
05501
05502 for (i=0; i<samparm->expct; i++)
05503 {
05504     strncpy(pbsamIn.exp[fil_][i], samparm->exp[fil][i], CHR_MAXLEN);
05505 }
05506
05507 // Running MSMS if the MSMS flag is used
05508 if (samparm->setmsms == 1) {
05509     for (i=0; i<pbamIn.nmol_; i++) {
05510         // find a clever way to use prefix of molecule name for msms outputs
05511         for (j=0; j < VMAX_ARGLEN; j++)
05512             if (nosh->molpath[i][j] == '\0') break;
05513
05514         // assume terminated by '.pqr' -> 4 char, want to term w/ '.xyzr'
05515         //char xyzr[j+2], surf[j+2], outname[j-4];
05516         char xyzr[VMAX_ARGLEN], surf[VMAX_ARGLEN], outname[VMAX_ARGLEN];
05517         for( k=0; k < j - 4; k++)
05518         {
05519             xyzr[k] = nosh->molpath[i][k];
05520             outname[k] = nosh->molpath[i][k];
05521             surf[k] = nosh->molpath[i][k];
05522         }
05523         outname[k] = '\0';
05524         xyzr[k] = '.'; surf[k] = '.';
05525         xyzr[k+1] = 'x'; surf[k+1] = 'v';
05526         xyzr[k+2] = 'y'; surf[k+2] = 'e';
05527         xyzr[k+3] = 'z'; surf[k+3] = 'r';

```

```
05527 xyzr[k+4] = 'r'; surf[k+4] = 't';
05528 xyzr[k+5] = '\0'; surf[k+5] = '\0';
05529
05530 // write an XYZR file from xyzr data
05531 FILE *fp;
05532 fp=fopen(xyzr, "w");
05533 Vatom *atom;
05534 for(k=0; k< Valist_getNumberAtoms(molecules[i]); k++)
05535 {
05536     atom = Valist_getAtom(molecules[i],k);
05537     fprintf(fp, "%.4f %.4f %.4f %.4f\n", Vatom_getPosition(atom)[0],
05538         Vatom_getPosition(atom)[1],
05539         Vatom_getPosition(atom)[2],
05540         Vatom_getRadius(atom));
05541 }
05542 fclose(fp);
05543
05544 #ifdef _WIN32
05545     sprintf(fname_tp, "msms.exe -if %s -prob %f -dens %f -of %s",
05546         xyzr, samparm->probe_radius, samparm->density, outname);
05547 #else
05548     sprintf(fname_tp, "msms -if %s -prob %f -dens %f -of %s",
05549         xyzr, samparm->probe_radius, samparm->density, outname);
05550 #endif
05551     printf("%s\n", fname_tp);
05552
05553     printf("Running MSMS...\n");
05554     ierr = system(fname_tp);
05555
05556     strncpy(pbsamIn.surffil_[i], surf, CHR_MAXLEN);
05557 }
05558 }
05559 }
05560
05561 // debug
05562 printPBSAMStruct( pbamIn, pbsamIn );
05563
05564 // Run the darn thing
05565 PBAMOutput pbamOut = runPBSAMWrapAPBS(pbamIn, pbsamIn, molecules, nosh->nmol);
05566
05567 Vnm_tprint(1, "\n\nReturning to APBS caller...\n\n");
05568
05569 if (!strcmp(pbamIn.runType_, "dynamics", 8) &&
05570     strcmp(pbamIn.runType_, "energyforce", 11)) {
05571     if (!strcmp(pbamIn.units_, "kcalmol", 7)) { //scale to kJmol is 4.18400
05572         Vnm_tprint(1, "Interaction energy in kCal/mol...\n\n");
05573         for (int i = 0; i < PBAMPARM_MAXMOL; i++) {
05574             Vnm_tprint(1, " Molecule %d: Global net ELEC energy = %1.12E\n",
05575                 i+1, pbamOut.energies_[i]);
05576             Vnm_tprint(1, " Force = (%1.6E, %1.6E, %1.6E)\n\n",
05577                 pbamOut.forces_[i][0], pbamOut.forces_[i][1],
05578                 pbamOut.forces_[i][2]);
05579             if (pbamOut.energies_[i+1] == 0.) break;
05580         }
05581     } else if (!strcmp(pbamIn.units_, "Jmol", 4)) { //scale to kJmol is 0.001
05582         Vnm_tprint(1, "Interaction energy in J/mol...\n\n");
05583         for (int i = 0; i < PBAMPARM_MAXMOL; i++) {
05584             Vnm_tprint(1, " Molecule %d: Global net ELEC energy = %1.12E\n",
05585                 i+1, pbamOut.energies_[i]);
05586             Vnm_tprint(1, " Force = (%1.6E, %1.6E, %1.6E)\n\n",
05587                 pbamOut.forces_[i][0], pbamOut.forces_[i][1],
05588                 pbamOut.forces_[i][2]);
05589             if (pbamOut.energies_[i+1] == 0.) break;
05590         }
05591     } else { // if (!strcmp(pbamIn.units_, "kT", 2)) //scale to kJmol is 2.478 @ 298K
05592         // or 0.008315436242 * 298
05593         Vnm_tprint(1, "Interaction energy in kT @ %6.2f K...\n\n", pbamIn.temp_);
05594         for (int i = 0; i < PBAMPARM_MAXMOL; i++) {
05595             Vnm_tprint(1, " Molecule %d: Global net ELEC energy = %1.12E\n",
05596                 i+1, pbamOut.energies_[i]);
05597             Vnm_tprint(1, " Force = (%1.6E, %1.6E, %1.6E)\n\n",
```

```

05608             pbamOut.forces_[i][0], pbamOut.forces_[i][1],
05609             pbamOut.forces_[i][2]);
05610         if (pbamOut.energies_[i+1] == 0.) break;
05611     }
05612 }
05613 }
05614
05615 Vnm_tstop(APBS_TIMER_SOLVER, "Solver timer");
05616
05617 return 1;
05618 }
05619
05620 #endif

```

9.152 src/routines.h File Reference

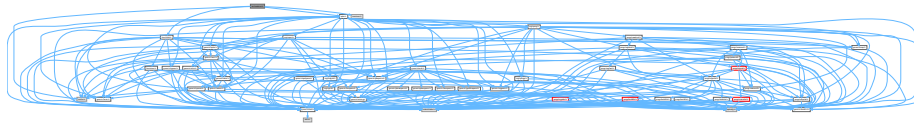
Header file for front end auxiliary routines.

```

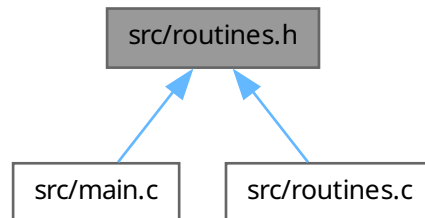
#include "apbs.h"
#include "mc/mc.h"
#include "fem/vfetk.h"
#include "mcx/mcx.h"

```

Include dependency graph for routines.h:



This graph shows which files directly or indirectly include this file:



Data Structures

- struct [AtomForce](#)
Structure to hold atomic forces.

Macros

- #define [APBSRC](#) 13
Return code for APBS during failure.

Typedefs

- typedef struct [AtomForce](#) [AtomForce](#)

Define [AtomForce](#) type.

Functions

- VEXTERNC [Vparam](#) * [loadParameter](#) ([NOsh](#) *nosh)
Loads and returns parameter object.
- VEXTERNC int [loadMolecules](#) ([NOsh](#) *nosh, [Vparam](#) *param, [Valist](#) *alist[[NOSH_MAXMOL](#)])
Load the molecules given in NOsh into atom lists.
- VEXTERNC void [killMolecules](#) ([NOsh](#) *nosh, [Valist](#) *alist[[NOSH_MAXMOL](#)])
Destroy the loaded molecules.
- VEXTERNC int [loadDielMaps](#) ([NOsh](#) *nosh, [Vgrid](#) *dielXMap[[NOSH_MAXMOL](#)], [Vgrid](#) *dielYMap[[NOSH_MAXMOL](#)], [Vgrid](#) *dielZMap[[NOSH_MAXMOL](#)])
Load the dielectric maps given in NOsh into grid objects.
- VEXTERNC void [killDielMaps](#) ([NOsh](#) *nosh, [Vgrid](#) *dielXMap[[NOSH_MAXMOL](#)], [Vgrid](#) *dielYMap[[NOSH_MAXMOL](#)], [Vgrid](#) *dielZMap[[NOSH_MAXMOL](#)])
Destroy the loaded dielectric.
- VEXTERNC int [loadKappaMaps](#) ([NOsh](#) *nosh, [Vgrid](#) *kappa[[NOSH_MAXMOL](#)])
Load the kappa maps given in NOsh into grid objects.
- VEXTERNC void [killKappaMaps](#) ([NOsh](#) *nosh, [Vgrid](#) *kappa[[NOSH_MAXMOL](#)])
Destroy the loaded kappa maps.
- VEXTERNC int [loadPotMaps](#) ([NOsh](#) *nosh, [Vgrid](#) *pot[[NOSH_MAXMOL](#)])
Load the potential maps given in NOsh into grid objects.
- VEXTERNC void [killPotMaps](#) ([NOsh](#) *nosh, [Vgrid](#) *pot[[NOSH_MAXMOL](#)])
Destroy the loaded potential maps.
- VEXTERNC int [loadChargeMaps](#) ([NOsh](#) *nosh, [Vgrid](#) *charge[[NOSH_MAXMOL](#)])
Load the charge maps given in NOsh into grid objects.
- VEXTERNC void [killChargeMaps](#) ([NOsh](#) *nosh, [Vgrid](#) *charge[[NOSH_MAXMOL](#)])
Destroy the loaded charge maps.
- VEXTERNC void [printPBEPARM](#) ([PBEparm](#) *pbeparm)
Print out generic PBE params loaded from input.
- VEXTERNC void [printMGPARAM](#) ([MGparm](#) *mgparm, double realCenter[3])
Print out MG-specific params loaded from input.
- VEXTERNC int [initMG](#) (int icalc, [NOsh](#) *nosh, [MGparm](#) *mgparm, [PBEparm](#) *pbeparm, double realCenter[3], [Vpbe](#) *pbe[[NOSH_MAXCALC](#)], [Valist](#) *alist[[NOSH_MAXMOL](#)], [Vgrid](#) *dielXMap[[NOSH_MAXMOL](#)], [Vgrid](#) *dielYMap[[NOSH_MAXMOL](#)], [Vgrid](#) *dielZMap[[NOSH_MAXMOL](#)], [Vgrid](#) *kappaMap[[NOSH_MAXMOL](#)], [Vgrid](#) *chargeMap[[NOSH_MAXMOL](#)], [Vpmgp](#) *pmgp[[NOSH_MAXCALC](#)], [Vpmg](#) *pmg[[NOSH_MAXCALC](#)], [Vgrid](#) *potMap[[NOSH_MAXMOL](#)])
Initialize an MG calculation.
- VEXTERNC void [killMG](#) ([NOsh](#) *nosh, [Vpbe](#) *pbe[[NOSH_MAXCALC](#)], [Vpmgp](#) *pmgp[[NOSH_MAXCALC](#)], [Vpmg](#) *pmg[[NOSH_MAXCALC](#)])
Kill structures initialized during an MG calculation.
- VEXTERNC int [solveMG](#) ([NOsh](#) *nosh, [Vpmg](#) *pmg, [MGparm_CalcType](#) type)
Solve the PBE with MG.
- VEXTERNC int [setPartMG](#) ([NOsh](#) *nosh, [MGparm](#) *mgparm, [Vpmg](#) *pmg)
Set MG partitions for calculating observables and performing I/O.

- VEXTERNC int [energyMG](#) ([NOsh](#) *nosh, int icalc, [Vpmg](#) *pmg, int *nenergy, double *totEnergy, double *qf←
Energy, double *qmEnergy, double *dielEnergy)
Calculate electrostatic energies from MG solution.
- VEXTERNC void [killEnergy](#) ()
Kill arrays allocated for energies.
- VEXTERNC int [forceMG](#) (Vmem *mem, [NOsh](#) *nosh, [PBEparm](#) *pbeparm, [MGparm](#) *mgparm, [Vpmg](#) *pmg, int
*nforce, [AtomForce](#) **atomForce, [Valist](#) *alist[[NOSH_MAXMOL](#)])
Calculate forces from MG solution.
- VEXTERNC void [killForce](#) (Vmem *mem, [NOsh](#) *nosh, int nforce[[NOSH_MAXCALC](#)], [AtomForce](#) *atom←
Force[[NOSH_MAXCALC](#)])
Free memory from MG force calculation.
- VEXTERNC void [storeAtomEnergy](#) ([Vpmg](#) *pmg, int icalc, double **atomEnergy, int *nenergy)
Store energy in arrays for future use.
- VEXTERNC int [writedataFlat](#) ([NOsh](#) *nosh, Vcom *com, const char *fname, double totEnergy[[NOSH_MAXCALC](#)],
double qfEnergy[[NOSH_MAXCALC](#)], double qmEnergy[[NOSH_MAXCALC](#)], double dielEnergy[[NOSH_MAXCALC](#)],
int nenergy[[NOSH_MAXCALC](#)], double *atomEnergy[[NOSH_MAXCALC](#)], int nforce[[NOSH_MAXCALC](#)],
[AtomForce](#) *atomForce[[NOSH_MAXCALC](#)])
Write out information to a flat file.
- VEXTERNC int [writedataXML](#) ([NOsh](#) *nosh, Vcom *com, const char *fname, double totEnergy[[NOSH_MAXCALC](#)],
double qfEnergy[[NOSH_MAXCALC](#)], double qmEnergy[[NOSH_MAXCALC](#)], double dielEnergy[[NOSH_MAXCALC](#)],
int nenergy[[NOSH_MAXCALC](#)], double *atomEnergy[[NOSH_MAXCALC](#)], int nforce[[NOSH_MAXCALC](#)],
[AtomForce](#) *atomForce[[NOSH_MAXCALC](#)])
Write out information to an XML file.
- VEXTERNC int [writedataMG](#) (int rank, [NOsh](#) *nosh, [PBEparm](#) *pbeparm, [Vpmg](#) *pmg)
Write out observables from MG calculation to file.
- VEXTERNC int [writematMG](#) (int rank, [NOsh](#) *nosh, [PBEparm](#) *pbeparm, [Vpmg](#) *pmg)
Write out operator matrix from MG calculation to file.
- VEXTERNC double [returnEnergy](#) (Vcom *com, [NOsh](#) *nosh, double totEnergy[[NOSH_MAXCALC](#)], int iprint)
Access net local energy.
- VEXTERNC int [printEnergy](#) (Vcom *com, [NOsh](#) *nosh, double totEnergy[[NOSH_MAXCALC](#)], int iprint)
Combine and pretty-print energy data (deprecated...see printElecEnergy)
- VEXTERNC int [printElecEnergy](#) (Vcom *com, [NOsh](#) *nosh, double totEnergy[[NOSH_MAXCALC](#)], int iprint)
Combine and pretty-print energy data.
- VEXTERNC int [printApolEnergy](#) ([NOsh](#) *nosh, int iprint)
Combine and pretty-print energy data.
- VEXTERNC int [printForce](#) (Vcom *com, [NOsh](#) *nosh, int nforce[[NOSH_MAXCALC](#)], [AtomForce](#) *atom←
Force[[NOSH_MAXCALC](#)], int i)
Combine and pretty-print force data (deprecated...see printElecForce)
- VEXTERNC int [printElecForce](#) (Vcom *com, [NOsh](#) *nosh, int nforce[[NOSH_MAXCALC](#)], [AtomForce](#) *atom←
Force[[NOSH_MAXCALC](#)], int i)
Combine and pretty-print force data.
- VEXTERNC int [printApolForce](#) (Vcom *com, [NOsh](#) *nosh, int nforce[[NOSH_MAXCALC](#)], [AtomForce](#) *atom←
Force[[NOSH_MAXCALC](#)], int i)
Combine and pretty-print force data.
- VEXTERNC void [startVio](#) ()
Wrapper to start MALOC Vio layer.
- VEXTERNC int [energyAPOL](#) ([APOLparm](#) *apolparm, double sasa, double sav, double atomsasa[], double
atomwcaEnergy[], int numatoms)
Calculate non-polar energies.

- VEXTERNC int **forceAPOL** (**Vacc** *acc, **Vmem** *mem, **APOLparm** *apolparm, int *nforce, **AtomForce** **atomForce, **Valist** *alist, **Vclist** *clist)

Calculate non-polar forces.
- VEXTERNC int **initAPOL** (**NOsh** *nosh, **Vmem** *mem, **Vparam** *param, **APOLparm** *apolparm, int *nforce, **AtomForce** **atomForce, **Valist** *alist)

Upperlevel routine to the non-polar energy and force routines.
- VEXTERNC void **printFEPARM** (int icalc, **NOsh** *nosh, **FEMparm** *feparm, **Vfetk** *fetk[NOSH_MAXCALC])

Print out FE-specific params loaded from input.
- VEXTERNC int **energyFE** (**NOsh** *nosh, int icalc, **Vfetk** *fetk[NOSH_MAXCALC], int *nenergy, double *totEnergy, double *qfEnergy, double *qmEnergy, double *dielEnergy)

Calculate electrostatic energies from FE solution.
- VPUBLIC Vrc_Codes **initFE** (int icalc, **NOsh** *nosh, **FEMparm** *feparm, **PBEparm** *pbeparm, **Vpbe** *pbe[NOSH_MAXCALC], **Valist** *alist[NOSH_MAXMOL], **Vfetk** *fetk[NOSH_MAXCALC])

Initialize FE solver objects.
- VEXTERNC void **killFE** (**NOsh** *nosh, **Vpbe** *pbe[NOSH_MAXCALC], **Vfetk** *fetk[NOSH_MAXCALC], **Gem** *gem[NOSH_MAXMOL])

Kill structures initialized during an FE calculation.
- VEXTERNC int **preRefineFE** (int i, **FEMparm** *feparm, **Vfetk** *fetk[NOSH_MAXCALC])

Pre-refine mesh before solve.
- VEXTERNC int **partFE** (int i, **NOsh** *nosh, **FEMparm** *feparm, **Vfetk** *fetk[NOSH_MAXCALC])

Partition mesh (if applicable)
- VEXTERNC int **solveFE** (int i, **PBEparm** *pbeparm, **FEMparm** *feparm, **Vfetk** *fetk[NOSH_MAXCALC])

Solve-estimate-refine.
- VEXTERNC int **postRefineFE** (int icalc, **FEMparm** *feparm, **Vfetk** *fetk[NOSH_MAXCALC])

Estimate error, mark mesh, and refine mesh after solve.
- VEXTERNC int **writedataFE** (int rank, **NOsh** *nosh, **PBEparm** *pbeparm, **Vfetk** *fetk)

Write FEM data to files.
- VEXTERNC Vrc_Codes **loadMeshes** (**NOsh** *nosh, **Gem** *gm[NOSH_MAXMOL])

Load the meshes given in NOsh into geometry objects.
- VEXTERNC void **killMeshes** (**NOsh** *nosh, **Gem** *alist[NOSH_MAXMOL])

Destroy the loaded meshes.

9.152.1 Detailed Description

Header file for front end auxiliary routines.

Author

Nathan Baker

Version

\$Id\$

Attention

```

*
* APBS -- Adaptive Poisson-Boltzmann Solver
*
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*
* Additional contributing authors listed in the code documentation.
*
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* THE POSSIBILITY OF SUCH DAMAGE.
*
*

```

Definition in file [routines.h](#).

9.153 routines.h

[Go to the documentation of this file.](#)

```

00001
00061 #ifndef _APBSROUTINES_H_
00062 #define _APBSROUTINES_H_
00063
00064 #include "apbs.h"
00065
00066 #ifdef HAVE_MC_H
00067 #   include "mc/mc.h"
00068 #   include "fem/vfetc.h"
00069 #endif
00070 #ifdef HAVE_MCX_H
00071 #   include "mcx/mcx.h"
00072 #endif
00073
00074 #ifdef ENABLE_BEM

```

```

00075  #include "TABIPBstruct.h"
00076 #endif
00077
00078 #ifdef ENABLE_GEOFLOW
00079  #include "GeometricFlowWrap.h"
00080 #endif
00081
00082 #if defined(ENABLE_PBAM) || defined(ENABLE_PBSAM)
00083  #include "PBAMWrap.h"
00084 #endif
00085
00086 #ifdef ENABLE_PBSAM
00087  #include "PBSAMWrap.h"
00088 #endif
00089
00093 #define APBSRC 13
00094
00099 struct AtomForce {
00100     double ibForce[3];
00101     double qfForce[3];
00102     double dbForce[3];
00103     double sasaForce[3];
00104     double savForce[3];
00105     double wcaForce[3];
00106 };
00107
00111 typedef struct AtomForce AtomForce;
00112
00118 VEXTERNC Vparam* loadParameter(
00119     Nosh *nosh
00121 );
00122
00128 VEXTERNC int loadMolecules(
00129     Nosh *nosh,
00130     Vparam *param,
00132     Valist *alist[NOSH_MAXMOL]
00134 );
00135
00142 VEXTERNC void killMolecules(Nosh *nosh, Valist *alist[NOSH_MAXMOL]);
00143
00153 VEXTERNC int loadDielMaps(Nosh *nosh,
00154     Vgrid *dielXMap[NOSH_MAXMOL],
00155     Vgrid *dielYMap[NOSH_MAXMOL],
00156     Vgrid *dielZMap[NOSH_MAXMOL]
00157 );
00158
00167 VEXTERNC void killDielMaps(Nosh *nosh, Vgrid *dielXMap[NOSH_MAXMOL],
00168     Vgrid *dielYMap[NOSH_MAXMOL], Vgrid *dielZMap[NOSH_MAXMOL]);
00169
00177 VEXTERNC int loadKappaMaps(Nosh *nosh, Vgrid *kappa[NOSH_MAXMOL]);
00178
00185 VEXTERNC void killKappaMaps(Nosh *nosh, Vgrid *kappa[NOSH_MAXMOL]);
00186
00194 VEXTERNC int loadPotMaps(Nosh *nosh, Vgrid *pot[NOSH_MAXMOL]);
00195
00202 VEXTERNC void killPotMaps(Nosh *nosh, Vgrid *pot[NOSH_MAXMOL]);
00203
00211 VEXTERNC int loadChargeMaps(Nosh *nosh, Vgrid *charge[NOSH_MAXMOL]);
00212
00219 VEXTERNC void killChargeMaps(Nosh *nosh, Vgrid *charge[NOSH_MAXMOL]);
00220
00226 VEXTERNC void printPBEPARM(PBEparm *pbeparm);
00227
00234 VEXTERNC void printMGPARAM(MGparm *mgparm, double realCenter[3]);
00235
00241 VEXTERNC int initMG(
00242     int icalc,
00243     Nosh *nosh,
00244     MGparm *mgparm,
00245     PBEparm *pbeparm,
00246     double realCenter[3],
00247     Vpbe *pbe[NOSH_MAXCALC],
00248     Valist *alist[NOSH_MAXMOL],
00249     Vgrid *dielXMap[NOSH_MAXMOL],
00250     Vgrid *dielYMap[NOSH_MAXMOL],
00251     Vgrid *dielZMap[NOSH_MAXMOL],
00252     Vgrid *kappaMap[NOSH_MAXMOL],
00253     Vgrid *chargeMap[NOSH_MAXMOL],
00254     Vpmgp *pmgp[NOSH_MAXCALC],
00255     Vpmg *pmg[NOSH_MAXCALC],
00256     Vgrid *potMap[NOSH_MAXMOL]

```



```

00257         );
00258
00264 VEXTERNC void killMG(
00265     Nosh *nosh,
00266     Vpbe *pbe[NOSH_MAXCALC],
00267     Vpmgp *pmgp[NOSH_MAXCALC],
00268     Vpmg *pmg[NOSH_MAXCALC]
00269 );
00270
00279 VEXTERNC int solveMG(Nosh *nosh, Vpmg *pmg, MGparm_CalcType type);
00280
00289 VEXTERNC int setPartMG(Nosh *nosh, MGparm *mgparm, Vpmg *pmg);
00290
00304 VEXTERNC int energyMG(Nosh *nosh, int icalc, Vpmg *pmg,
00305     int *nenergy, double *totEnergy, double *qfEnergy, double *qmEnergy,
00306     double *dielEnergy);
00307
00312 VEXTERNC void killEnergy();
00313
00327 VEXTERNC int forceMG(Vmem *mem, Nosh *nosh, PBEparm *pbeparm, MGparm *mgparm,
00328     Vpmg *pmg, int *nforce, AtomForce **atomForce, Valist *alist[NOSH_MAXMOL]);
00329
00338 VEXTERNC void killForce(Vmem *mem, Nosh *nosh, int nforce[NOSH_MAXCALC],
00339     AtomForce *atomForce[NOSH_MAXCALC]);
00340
00345 VEXTERNC void storeAtomEnergy(
00346     Vpmg *pmg,
00347     int icalc,
00348     double **atomEnergy,
00349     int *nenergy
00350 );
00351
00368 VEXTERNC int writedataFlat(Nosh *nosh, Vcom *com, const char *fname,
00369     double totEnergy[NOSH_MAXCALC], double qfEnergy[NOSH_MAXCALC],
00370     double qmEnergy[NOSH_MAXCALC], double dielEnergy[NOSH_MAXCALC],
00371     int nenergy[NOSH_MAXCALC], double *atomEnergy[NOSH_MAXCALC],
00372     int nforce[NOSH_MAXCALC], AtomForce *atomForce[NOSH_MAXCALC]);
00373
00390 VEXTERNC int writedataXML(Nosh *nosh, Vcom *com, const char *fname,
00391     double totEnergy[NOSH_MAXCALC], double qfEnergy[NOSH_MAXCALC],
00392     double qmEnergy[NOSH_MAXCALC], double dielEnergy[NOSH_MAXCALC],
00393     int nenergy[NOSH_MAXCALC], double *atomEnergy[NOSH_MAXCALC],
00394     int nforce[NOSH_MAXCALC], AtomForce *atomForce[NOSH_MAXCALC]);
00395
00405 VEXTERNC int writedataMG(int rank, Nosh *nosh, PBEparm *pbeparm, Vpmg *pmg);
00406
00416 VEXTERNC int writematMG(int rank, Nosh *nosh, PBEparm *pbeparm, Vpmg *pmg);
00417
00427 VEXTERNC double returnEnergy(Vcom *com, Nosh *nosh, double totEnergy[NOSH_MAXCALC], int iprint);
00428
00434 VEXTERNC int printEnergy(
00435     Vcom *com,
00436     Nosh *nosh,
00437     double totEnergy[NOSH_MAXCALC],
00438     int iprint
00439 );
00440
00441
00447 VEXTERNC int printElecEnergy(
00448     Vcom *com,
00449     Nosh *nosh,
00450     double totEnergy[NOSH_MAXCALC],
00451     int iprint
00452 );
00453
00454
00460 VEXTERNC int printApolEnergy(
00461     Nosh *nosh,
00462     int iprint
00463 );
00464
00470 VEXTERNC int printForce(
00471     Vcom *com,
00472     Nosh *nosh,
00473     int nforce[NOSH_MAXCALC],
00474     AtomForce *atomForce[NOSH_MAXCALC],
00475     int i
00476 );
00477
00483 VEXTERNC int printElecForce(
00484     Vcom *com,
00485     Nosh *nosh,
00486     int nforce[NOSH_MAXCALC],

```

```

00487             AtomForce *atomForce[NOSH_MAXCALC],
00488             int i
00489             );
00490
00496 VEXTERNC int printApolForce(
00497             Vcom *com,
00498             Nosh *nosh,
00499             int nforce[NOSH_MAXCALC],
00500             AtomForce *atomForce[NOSH_MAXCALC],
00501             int i
00502             );
00503
00508 VEXTERNC void startVio();
00509
00515 VEXTERNC int energyAPOL(
00516             APOLparm *apolparm,
00517             double sasa,
00518             double sav,
00519             double atomsasa[],
00520             double atomwcaEnergy[],
00521             int numatoms
00522             );
00523
00529 VEXTERNC int forceAPOL(
00530             Vacc *acc,
00531             Vmem *mem,
00532             APOLparm *apolparm,
00533             int *nforce,
00534             AtomForce **atomForce,
00535             Valist *alist,
00536             Vclist *clist
00537             );
00538
00547 VEXTERNC int initAPOL(
00548             Nosh *nosh,
00549             Vmem *mem,
00550             Vparam *param,
00551             APOLparm *apolparm,
00552             int *nforce,
00553             AtomForce **atomForce,
00554             Valist *alist
00555             );
00556
00557
00558 #ifdef HAVE_MC_H
00559 #include "fem/vfetc.h"
00560
00569 VEXTERNC void printFEPARM(int icalc, Nosh *nosh, FEParm *feparm,
00570             Vfetc *fetc[NOSH_MAXCALC]);
00571
00586 VEXTERNC int energyFE(Nosh* nosh, int icalc, Vfetc *fetc[NOSH_MAXCALC],
00587             int *nenergy, double *totEnergy, double *qfEnergy, double *qmEnergy,
00588             double *dielEnergy);
00589
00597 VEXTERNC Vrc_Codes initFE(
00598             int icalc,
00599             Nosh *nosh,
00600             FEParm *feparm,
00601             PBEParm *pbeparm,
00602             Vpbe *pbe[NOSH_MAXCALC],
00603             Valist *alist[NOSH_MAXMOL],
00604             Vfetc *fetc[NOSH_MAXCALC]
00605             );
00606
00612 VEXTERNC void killFE(
00613             Nosh *nosh,
00614             Vpbe *pbe[NOSH_MAXCALC],
00615             Vfetc *fetc[NOSH_MAXCALC],
00616             Gem *gem[NOSH_MAXMOL]
00617             );
00618
00628 VEXTERNC int preRefineFE(int i,
00629             FEParm *feparm,
00630             Vfetc *fetc[NOSH_MAXCALC]
00631             );
00632
00642 VEXTERNC int partFE(int i, Nosh *nosh, FEParm *feparm,
00643             Vfetc *fetc[NOSH_MAXCALC]);
00644
00654 VEXTERNC int solveFE(int i,
00655             PBEParm *pbeparm,

```

```
00656             FEMparm *feparm,
00657             Vfetk *fetk[NOSH_MAXCALC]
00658 );
00659
00671 VEXTERNC int postRefineFE(int icalc,
00672             FEMparm *feparm,
00673             Vfetk *fetk[NOSH_MAXCALC]
00674 );
00675
00685 VEXTERNC int writedataFE(int rank, NOSH *nosh, PBEparm *pbeparm, Vfetk *fetk);
00686
00692 VEXTERNC Vrc_Codes loadMeshes(
00693             NOSH *nosh,
00694             Gem *gm[NOSH_MAXMOL]
00695 );
00696
00702 VEXTERNC void killMeshes(
00703             NOSH *nosh,
00704             Gem *alist[NOSH_MAXMOL]
00705 );
00706 #endif
00707 #endif
00708 #endif
00709
00710
00711
00712 VEXTERNC void printMGPARAM(MGparm *mgparm, double realCenter[3]);
00713
00714 #ifdef ENABLE_BEM
00720 VEXTERNC int initBEM(
00721             int icalc,
00722             NOSH *nosh,
00723             BEMparm *beparm,
00724             PBEparm *pbeparm,
00725             Vpbe *pbe[NOSH_MAXCALC]
00726 );
00727
00733 VEXTERNC void killBEM(
00734             NOSH *nosh,
00735             Vpbe *pbe[NOSH_MAXCALC]
00736 );
00737
00746 VEXTERNC int solveBEM(Valist* molecules[NOSH_MAXMOL], NOSH *nosh, PBEparm *pbeparm, BEMparm *beparm,
00747             BEMparm_CalcType type);
00748
00756 VEXTERNC int setPartBEM(NOSH *nosh, BEMparm *beparm);
00757
00771 VEXTERNC int energyBEM(NOSH* nosh, int icalc,
00772             int *nenergy, double *totEnergy, double *qfEnergy, double *qmEnergy,
00773             double *dielEnergy);
00774
00788 VEXTERNC int forceBEM(NOSH *nosh, PBEparm *pbeparm, BEMparm *beparm,
00789             int *nforce, AtomForce **atomForce, Valist *alist[NOSH_MAXMOL]);
00790
00797 VEXTERNC void printBEMPARAM(BEMparm *beparm);
00798
00808 VEXTERNC int writedataBEM(int rank, NOSH *nosh, PBEparm *pbeparm);
00809
00819 VEXTERNC int writematBEM(int rank, NOSH *nosh, PBEparm *pbeparm);
00820 #endif
00821
00822 #ifdef ENABLE_GEOFLOW
00830 VEXTERNC int solveGeometricFlow(
00831             Valist* molecules[NOSH_MAXMOL],
00832             NOSH *nosh,
00833             PBEparm *pbeparm,
00834             APOLparm *apolparm,
00835             GEOFLOWparm *parm
00836 );
00837 #endif
00838
00839 #ifdef ENABLE_PBAM
00847 VEXTERNC int solvePBAM(
00848             Valist* molecules[NOSH_MAXMOL],
00849             NOSH *nosh,
00850             PBEparm *pbeparm,
00851             PBAMparm *parm
00852 );
00853 #endif
00854
00855 #ifdef ENABLE_PBSAM
```

```
00863 VEXTERNC int solvePBSAM(  
00864     Valist* molecules[NOSH_MAXMOL],  
00865     Nosh *nosh,  
00866     PBEparm *pbeparm,  
00867     PBAMparm *parm,  
00868     PBSAMparm *samparm  
00869 );  
00870 #endif
```

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