iAPBS

2.1.0

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1.1 Directories

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2.1 File List

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Chapter 3

Directory Documentation

3.1 /home/rok/SB.new/b/apbs/contrib/iapbs/src/ Directory Reference

Files

- file apbs_driver.c

  The main iAPBS driver code.

- file apbs_driver.h

  Header file for the main iAPBS driver.

- file **wrapper.f**
- file **wrapper_inc.f**

Chapter 4

File Documentation

4.1 apbs_driver.c File Reference

The main iAPBS driver code.

```
#include "apbs/apbs.h"
#include "apbs/nosh.h"
#include "apbs/mgparm.h"
#include "apbs/pbeparm.h"
#include "apbs/femparm.h"
#include "apbs/routines.h"
#include "apbs_driver.h"
```

Defines

- #define MAX_BUF_SIZE 4096

  Buffer size for internal APBS string input.

Functions

- int apbsdrv_ (int *nat, double x[NATOMS], double y[NATOMS], double z[NATOMS], double radius[NATOMS], double charge[NATOMS], double r_param[9], int i_param[25], double grid[3], int dime[3], int pdime[3], double glen[3], double center[3], double cglen[3], double fglen[3], double ccenter[3],

double fcenter[3], double *ofrac, int *dbg, double ionq[MAXION], double ionc[MAXION], double ionr[MAXION], double esenergy[1], double npenergy[1], double apbsdx[NATOMS], double apbsdy[NATOMS], double apbsdz[NATOMS], double apbsqfx[NATOMS], double apbsqfy[NATOMS], double apbsqfz[NATOMS], double apbsibx[NATOMS], double apbsiby[NATOMS], double apbsibz[NATOMS], double apbsnpx[NATOMS], double apbsnpy[NATOMS], double apbsnpz[NATOMS], double apbsdbx[NATOMS], double apbsdby[NATOMS], double apbsdbz[NATOMS])

Wrapper iAPBS function.

- char * setupString (double r_param[9], int i_param[25], double grid[3], int dime[3], double ionq[MAXION], double ionc[MAXION], double ionr[MAXION], double glen[3], double center[3], double cglen[3], double fglen[3], double ccenter[3], double fcenter[3], double *ofrac, int pdime[3], int debug)

  Creates APBS input string.

- double getElecEnergy (Vcom *com, NOsh *nosh, double totEnergy[NOSH_MAXCALC], int iprint)

  Combine and pretty-print energy data.

4.1.1 Detailed Description

The main iAPBS driver code.

Author

Robert Konecny

Note

Energy is returned in kJ/mol, forces in kJ/(mol/A).

Revision

556

Id

apbs_driver.c 556 2012-01-10 03:03:33Z rok

4.1.2 Function Documentation

4.1.2.1 int apbsdrv_ (int * *nat*, double *x*[NATOMS], double *y*[NATOMS], double *z*[NATOMS], double *radius*[NATOMS], double *charge*[NATOMS], double *r_param*[9], int *i_param*[25], double *grid*[3], int *dime*[3], int *pdime*[3], double *glen*[3], double *center*[3], double *cglen*[3], double *fglen*[3], double *ccenter*[3], double *fcenter*[3], double * *ofrac*, int * *dbg*, double *ionq*[MAXION], double *ionc*[MAXION], double *ionr*[MAXION], double *esenergy*[1], double *npenergy*[1], double *apbsdx*[NATOMS], double *apbsdy*[NATOMS], double *apbsdz*[NATOMS], double *apbsqfx*[NATOMS], double *apbsqfy*[NATOMS], double *apbsqfz*[NATOMS], double *apbsibx*[NATOMS], double *apbsiby*[NATOMS], double *apbsibz*[NATOMS], double *apbsnpx*[NATOMS], double *apbsnpy*[NATOMS], double *apbsnpz*[NATOMS], double *apbsdbx*[NATOMS], double *apbsdby*[NATOMS], double *apbsdbz*[NATOMS])

Wrapper iAPBS function.

Author

Robert Konecny

References getElecEnergy(), MAX_BUF_SIZE, and setupString().

4.1.2.2 double getElecEnergy (Vcom * *com*, NOsh * *nosh*, double *totEnergy*[NOSH_MAXCALC], int *iprint*)

Combine and pretty-print energy data.

Note

Collect Elect Energy

Author

Robert Konecny

Parameters

nosh Communications object

totEnergy Parameters from input file

iprint Array of energies from different calculations Index of energy statement to print

Referenced by apbsdrv_().

4.1.2.3 char* setupString (double *r_param*[9], int *i_param*[25], double *grid*[3], int *dime*[3], double *ionq*[MAXION], double *ionc*[MAXION], double *ionr*[MAXION], double *glen*[3], double *center*[3], double *cglen*[3], double *fglen*[3], double *ccenter*[3], double *fcenter*[3], double * *ofrac*, int *pdime*[3], int *debug*)

Creates APBS input string.

Author

Robert Konecny

References MAX_BUF_SIZE.

Referenced by apbsdrv_().

4.2 apbs_driver.h File Reference

Header file for the main iAPBS driver.

Defines

- #define NATOMS 150000

  Maximum number of atoms.

Functions

- VEXTERNC int apbsdrv_ (int *nat, double x[NATOMS], double y[NATOMS], double z[NATOMS], double radius[NATOMS], double charge[NATOMS], double r_param[9], int i_param[25], double grid[3], int dime[3], int pdime[3], double glen[3], double center[3], double cglen[3], double fglen[3], double ccenter[3], double fcenter[3], double *ofrac, int *dbg, double ionq[MAXION], double ionc[MAXION], double ionr[MAXION], double esEnergy[NOSH_MAXCALC], double npEnergy[NOSH_MAXCALC], double apbsdx[NATOMS], double apbsdy[NATOMS], double apbsdz[NATOMS], double apbsqfx[NATOMS], double apbsqfy[NATOMS], double apbsqfz[NATOMS], double apbsibx[NATOMS], double apbsiby[NATOMS], double apbsibz[NATOMS], double apbsnpx[NATOMS], double apbsnpy[NATOMS], double apbsnpz[NATOMS], double apbsdbx[NATOMS], double apbsdby[NATOMS], double apbsdbz[NATOMS])

  Wrapper iAPBS function.

- VEXTERNC int iforceMG (Vmem *mem, NOsh *nosh, PBEparm *pbeparm, MGparm *mgparm, Vpmg *pmg, int *nforce, AtomForce **atomForce, Valist *alist[NOSH_MAXMOL], int debug)

  Calculate forces from MG solution.

- double getElecEnergy (Vcom *com, NOsh *nosh, double totEnergy[NOSH_MAXCALC], int iprint)

  Combine and pretty-print energy data.

- char * setupString (double r_param[9], int i_param[25], double grid[3], int dime[3], double ionq[MAXION], double ionc[MAXION], double ionr[MAXION], double glen[3], double center[3], double cglen[3], double fglen[3], double ccenter[3], double fcenter[3], double *ofrac, int pdime[3], int debug)

  Creates APBS input string.

4.2.1 Detailed Description

Header file for the main iAPBS driver.

Author

Robert Konecny

Version

Id

apbs_driver.h 389 2010-03-29 20:18:15Z rok

4.2.2 Function Documentation

4.2.2.1 VEXTERNC int apbsdrv_ (int * *nat*, double *x*[NATOMS], double *y*[NATOMS], double *z*[NATOMS], double *radius*[NATOMS], double *charge*[NATOMS], double *r_param*[9], int *i_param*[25], double *grid*[3], int *dime*[3], int *pdime*[3], double *glen*[3], double *center*[3], double *cglen*[3], double *fglen*[3], double *ccenter*[3], double *fcenter*[3], double * *ofrac*, int * *dbg*, double *ionq*[MAXION], double *ionc*[MAXION], double *ionr*[MAXION], double *esEnergy*[NOSH_MAXCALC], double *npEnergy*[NOSH_MAXCALC], double *apbsdx*[NATOMS], double *apbsdy*[NATOMS], double *apbsdz*[NATOMS], double *apbsqfx*[NATOMS], double *apbsqfy*[NATOMS], double *apbsqfz*[NATOMS], double *apbsibx*[NATOMS], double *apbsiby*[NATOMS], double *apbsibz*[NATOMS], double *apbsnpx*[NATOMS], double *apbsnpy*[NATOMS], double *apbsnpz*[NATOMS], double *apbsdbx*[NATOMS], double *apbsdby*[NATOMS], double *apbsdbz*[NATOMS])

Wrapper iAPBS function.

Author

Robert Konecny

Parameters

nat Number of atoms

x Atomic coordinate (x)

y Atomic coordinate (y)

z Atomic coordinate (z)

radius Atomic radii
charge Atomic charges
r_param Input APBS parameters (real values)
i_param Input APBS parameters (integer values)
grid Grid spacing
dime Grid dimensions
pdime Grid of processors to be used in calculation
glen Grid side lengths
center Grid center
cglen Coarse grid side lengths
fglen Fine grid side lengths
ccenter Coarse grid center
fcenter Fine grid center
ofrac Overlap fraction between procs
dbg Debug verbosity flag
ionq Mobile ion charge
ionc Mobile ion concentration
ionr Mobile ion radius
esEnergy Electrostatic energy
npEnergy Non-polar energy
apbsdx Total electrostatic force per atom (x coordinate)
apbsdy Total electrostatic force per atom (y coordinate)
apbsdz Total electrostatic force per atom (z coordinate)
apbsqfx Fixed charge force (x)
apbsqfy Fixed charge force (y)
apbsqfz Fixed charge force (z)
apbsibx Ionic boundary force (x)
apbsiby Ionic boundary force (y)
apbsibz Ionic boundary force (z)
apbsnpx Non-polar force (x)
apbsnpy Non-polar force (y)
apbsnpz Non-polar force (z)
apbsdbx Dielectric boundary force (x)
apbsdby Dielectric boundary force (y)
apbsdbz Dielectric boundary force (z)

Returns

1 if successful, 0 otherwise

4.2.2.2 double getElecEnergy (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

Note

Collect Elect Energy

Author

Robert Konecny

Parameters

nosh Communications object

totEnergy Parameters from input file

iprint Array of energies from different calculations Index of energy statement to print

Referenced by apbsdrv_().

4.2.2.3 VEXTERNC int iforceMG (Vmem * *mem*, NOsh * *nosh*, PBEparm * *pbeparm*, MGparm * *mgparm*, Vpmg * *pmg*, int * *nforce*, AtomForce ** *atomForce*, Valist * *alist*[NOSH_MAXMOL], int *debug*)

Calculate forces from MG solution.

Author

Robert Konecny (based on forceMG)

Parameters

mem Memory management object

nosh Parameters from input file

pbeparm Generic PBE parameters

mgparm MG-specific parmaeters

pmg MG object

nforce 0 => no forces, 1 => net forces, >1 => number of forces (1 per atom)

atomForce Pointer to array of force objects

alist List of atom lists

debug verbosity flag

Returns

1 if successful, 0 otherwise

4.2.2.4 char* setupString (double *r_param*[9], int *i_param*[25], double *grid*[3], int *dime*[3], double *ionq*[MAXION], double *ionc*[MAXION], double *ionr*[MAXION], double *glen*[3], double *center*[3], double *cglen*[3], double *fglen*[3], double *ccenter*[3], double *fcenter*[3], double * *ofrac*, int *pdime*[3], int *debug*)

Creates APBS input string.

Author

Robert Konecny

Parameters

r_param Input APBS parameters (real values)

i_param Input APBS parameters (integer values)

grid Grid spacing

dime Grid dimensions

ionq Mobile ion charge

ionc Mobile ion concentration

ionr Mobile ion radius

glen Grid side lengths

center Grid center

cglen Coarse grid side lengths

fglen Fine grid side lengths

ccenter Coarse grid center

fcenter Fine grid center

ofrac Overlap fraction between procs

pdime Grid of processors to be used in calculation

debug Debug verbosity level.

Returns

the input string

Author

Robert Konecny

References MAX_BUF_SIZE.

Referenced by apbsdrv_().

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