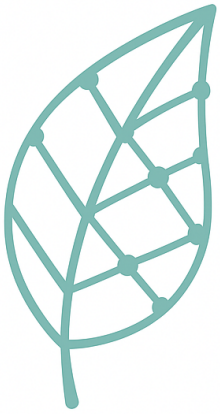

Lamina

Lemina

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Chapter 1

Lemina

Chapter 2

File Index

2.1 File List

Here is a list of all files with brief descriptions:

Chapter 3

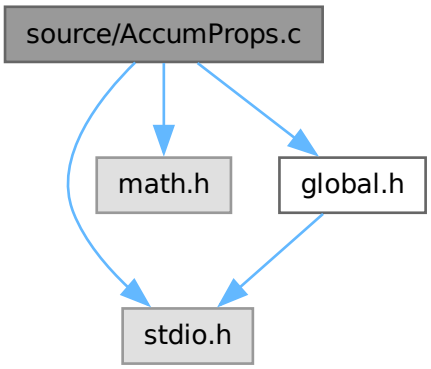
File Documentation

3.1 README.md File Reference

3.2 source/AccumProps.c File Reference

```
#include <stdio.h>
#include <math.h>
#include "global.h"
```

Include dependency graph for AccumProps.c:



Functions

- void AccumProps (int icode)

3.2.1 Function Documentation

3.2.1.1 AccumProps()

```
void AccumProps (
            int icode )
```

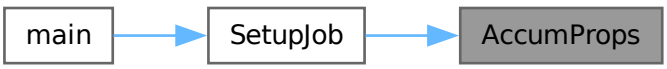
Definition at line 25 of file AccumProps.c.

```
00025                           {
00026  if(icode == 0){
00027  sPotEnergy = ssPotEnergy = 0.;
00028  sKinEnergy = ssKinEnergy = 0.;
00029  sPressure = ssPressure = 0.;
00030  sTotEnergy = ssTotEnergy = 0.;
00031  svirSum = 0.;
00032  }else if(icode == 1){
00033  sPotEnergy += potEnergy;
00034  ssPotEnergy += Sqr(potEnergy);
00035  sKinEnergy += kinEnergy;
00036  ssKinEnergy += Sqr(kinEnergy);
00037  sTotEnergy += totEnergy;
00038  ssTotEnergy += Sqr(totEnergy);
00039  sPressure += pressure;
00040  ssPressure += Sqr(pressure);
00041  svirSum += virSum;
00042  }else if(icode == 2){
00043  sPotEnergy /= stepAvg;
00044  ssPotEnergy /= sqrt(ssPotEnergy/stepAvg - Sqr(sPotEnergy));
00045  sTotEnergy /= stepAvg;
00046  ssTotEnergy = sqrt(ssTotEnergy/stepAvg - Sqr(sTotEnergy));
00047  sKinEnergy /= stepAvg;
00048  ssKinEnergy = sqrt(ssKinEnergy/stepAvg - Sqr(sKinEnergy));
00049  sPressure /= stepAvg;
00050  ssPressure = sqrt(ssPressure/stepAvg - Sqr(sPressure));
00051  svirSum /= stepAvg;
00052  } }
```

References kinEnergy, potEnergy, pressure, sKinEnergy, sPotEnergy, sPressure, Sqr, ssKinEnergy, ssPotEnergy, ssPressure, ssTotEnergy, stepAvg, sTotEnergy, svirSum, totEnergy, and virSum.

Referenced by SetupJob().

Here is the caller graph for this function:



3.3 AccumProps.c

Go to the documentation of this file.

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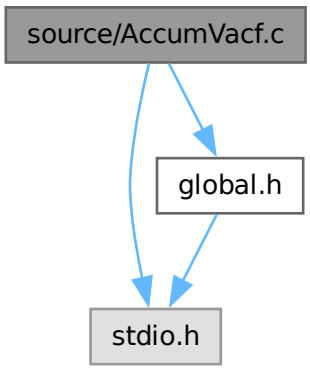
00016
00017  Copyright (C) 2025 Harish Charan, University of Durham, UK
00018
00019  */
00020
00021 #include<stdio.h>
00022 #include<math.h>
00023 #include"global.h"
00024
00025 void AccumProps(int icode){
00026  if(icode == 0){
00027  sPotEnergy = ssPotEnergy = 0.;
00028  sKinEnergy = ssKinEnergy = 0.;
00029  sPressure = ssPressure = 0.;
00030  sTotEnergy = ssTotEnergy = 0.;
00031  svirSum = 0.;
00032  }else if(icode == 1){
00033  sPotEnergy += potEnergy;
00034  ssPotEnergy += Sqr(potEnergy);
00035  sKinEnergy += kinEnergy;
00036  ssKinEnergy += Sqr(kinEnergy);
00037  sTotEnergy += totEnergy;
00038  ssTotEnergy += Sqr(totEnergy);
00039  sPressure += pressure;
00040  ssPressure += Sqr(pressure);
00041  svirSum += virSum;
00042  }else if(icode == 2){
00043  sPotEnergy /= stepAvg;
00044  ssPotEnergy /= sqrt(ssPotEnergy/stepAvg - Sqr(sPotEnergy));
00045  sTotEnergy /= stepAvg;
00046  ssTotEnergy = sqrt(ssTotEnergy/stepAvg - Sqr(sTotEnergy));
00047  sKinEnergy /= stepAvg;
00048  ssKinEnergy = sqrt(ssKinEnergy/stepAvg - Sqr(sKinEnergy));
00049  sPressure /= stepAvg;
00050  ssPressure = sqrt(ssPressure/stepAvg - Sqr(sPressure));
00051  svirSum /= stepAvg;
00052  } }
```

3.4 source/AccumVacf.c File Reference

```
#include <stdio.h>
#include "global.h"
```

Include dependency graph for AccumVacf.c:



Functions

- double Integrate (double *, int)
- void PrintVacf ()
- void ZeroVacf ()
- void AccumVacf ()

3.4.1 Function Documentation

3.4.1.1 AccumVacf()

```
void AccumVacf ( )
```

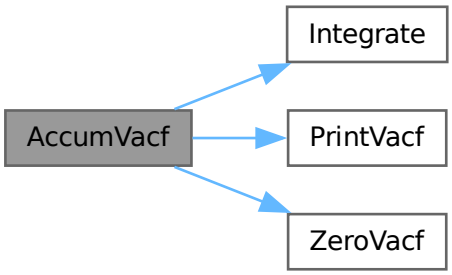
Definition at line 27 of file AccumVacf.c.

```
00027                  {
00028  double fac;
00029  int j, nb;
00030  for(nb = 1 ; nb <= nBuffAcf ; nb ++){
00031   if(indexAcf[nb] == nValAcf){
00032    for(j = 1 ; j <= nValAcf; j ++){
00033     viscAcfAv[j] +=  viscAcf[nb][j];
00034     }
00035   indexAcf[nb] = 0;
00036   countAcfAv ++;
00037   if(countAcfAv == limitAcfAv){
00038    fac = 1./(kinEnergy*region[1]*region[2]*limitAcfAv);
00039    viscAcfInt = fac*stepAcf*deltaT*Integrate(viscAcfAv, nValAcf);
00040    PrintVacf();
00041    ZeroVacf();
00042 } } } }
```

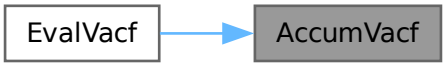
References countAcfAv, deltaT, indexAcf, Integrate(), kinEnergy, limitAcfAv, nBuffAcf, nValAcf, PrintVacf(), region, stepAcf, viscAcf, viscAcfAv, viscAcfInt, and ZeroVacf().

Referenced by EvalVacf().

Here is the call graph for this function:



Here is the caller graph for this function:



3.4.1.2 Integrate()

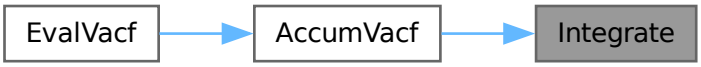
```
double Integrate (
            double * f,
            int nf )
```

Definition at line 25 of file Integrate.c.

```
00025                                   {
00026  double s;
00027  int i;
00028  s = 0.5*(f[1] + f[nf]);
00029  for(i = 2 ; i <= nf - 1 ; i ++)
00030   s += f[i];
00031  return(s);
00032 }
```

Referenced by AccumVacf().

Here is the caller graph for this function:



3.4.1.3 PrintVacf()

```
void PrintVacf ( )
```

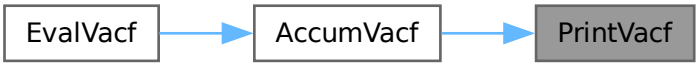
Definition at line 25 of file PrintVacf.c.

```
00025                 {
00026  double tVal;
00027  int j;
00028  fprintf(fpvisc,"viscosity acf\n");
00029  for(j = 1 ; j <= nValAcf ; j ++){
00030   tVal = (j-1)*stepAcf*deltaT;
00031   fprintf(fpvisc, "%lf\t %lf\t %lf\n", tVal, viscAcfAv[j], viscAcfAv[j]/viscAcfAv[1]);
00032   }
00033  fprintf(fpvisc, "viscosity acf integral : %lf\n", viscAcfInt);
00034 }
```

References deltaT, fpvisc, nValAcf, stepAcf, viscAcfAv, and viscAcfInt.

Referenced by AccumVacf().

Here is the caller graph for this function:



3.4.1.4 ZeroVacf()

```
void ZeroVacf ( )
```

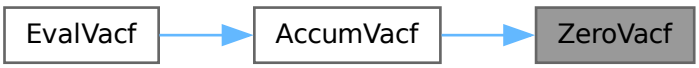
Definition at line 25 of file ZeroVacf.c.

```
00025                {
00026  int j;
00027  countAcfAv= 0 ;
00028  for(j = 1 ; j <= nValAcf ; j ++)
00029   viscAcfAv[j] = 0.;
00030 }
```

References countAcfAv, nValAcf, and viscAcfAv.

Referenced by AccumVacf().

Here is the caller graph for this function:



3.5 AccumVacf.c

Go to the documentation of this file.

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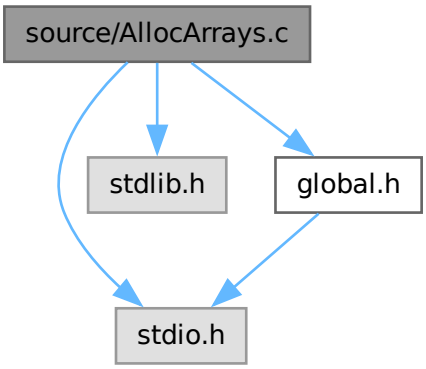
00016
00017  Copyright (C) 2025 Harish Charan, University of Durham, UK
00018
00019  */
00020
00021 #include<stdio.h>
00022 #include"global.h"
00023
00024 double Integrate(double *, int);
00025  void PrintVacf();
00026  void ZeroVacf();
00027  void AccumVacf(){
00028  double fac;
00029  int j, nb;
00030  for(nb = 1 ; nb <= nBuffAcf ; nb ++){
00031   if(indexAcf[nb] == nValAcf){
00032    for(j = 1 ; j <= nValAcf; j ++){
00033     viscAcfAv[j] +=  viscAcf[nb][j];
00034     }
00035   indexAcf[nb] = 0;
00036   countAcfAv ++;
00037   if(countAcfAv == limitAcfAv){
00038    fac = 1./(kinEnergy*region[1]*region[2]*limitAcfAv);
00039    viscAcfInt = fac*stepAcf*deltaT*Integrate(viscAcfAv, nValAcf);
00040    PrintVacf();
00041    ZeroVacf();
00042 } } } }
00043
```

3.6 source/AllocArrays.c File Reference

```
#include <stdio.h>
#include <stdlib.h>
#include "global.h"
```

Include dependency graph for AllocArrays.c:



Functions

- void AllocArrays ()

3.6.1 Function Documentation

3.6.1.1 AllocArrays()

```
void AllocArrays ( )
```

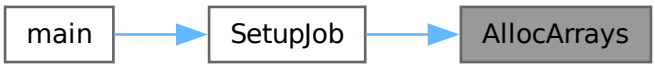
Definition at line 25 of file AllocArrays.c.

```
00025                   {
00026  int n;
00027  // SPACETIME CORRELATIONS
00028  cfOrg = (double **) malloc ((nBuffCorr+1)*sizeof(double *));
00029  for (n = 0; n <= nBuffCorr; n++)
00030   cfOrg[n] = (double *) malloc ((2*nFunCorr+1)*sizeof(double));
00031
00032  cfVal = (double *) malloc ((2*nFunCorr+1)*sizeof(double));
00033  indexCorr = (int *) malloc ((nBuffCorr+1)*sizeof(int));
00034
00035  spacetimeCorr = (double **) malloc ((nBuffCorr+1)*sizeof(double));
00036  for (n = 0; n <= nBuffCorr; n++)
00037  spacetimeCorr[n] = (double *) malloc ((nFunCorr*nValCorr+1)*sizeof(double));
00038
00039  spacetimeCorrAv = (double *) malloc ((nFunCorr*nValCorr+1)*sizeof(double));
00040  // VISCOSITY
00041  indexAcf = (double *)malloc((nBuffAcf+1)*sizeof(double));
00042  viscAcf = (double **)malloc((nBuffAcf+1)*sizeof(double *));
00043  for(n = 0 ; n <= nBuffAcf ; n ++)
00044   viscAcf[n] = (double *)malloc((nValAcf+1)*sizeof(double ));
00045
00046  viscAcfOrg = (double *)malloc((nBuffAcf+1)*sizeof(double));
00047  viscAcfAv = (double *)malloc((nValAcf+1)*sizeof(double));
00048
00049   // RDF
00050   histRdf = (double *)malloc((sizeHistRdf+1)*sizeof(double));
00051 }
```

References cfOrg, cfVal, histRdf, indexAcf, indexCorr, nBuffAcf, nBuffCorr, nFunCorr, nValAcf, nValCorr, sizeHistRdf, spacetimeCorr, spacetimeCorrAv, viscAcf, viscAcfAv, and viscAcfOrg.

Referenced by SetupJob().

Here is the caller graph for this function:



3.7 AllocArrays.c

Go to the documentation of this file.

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```

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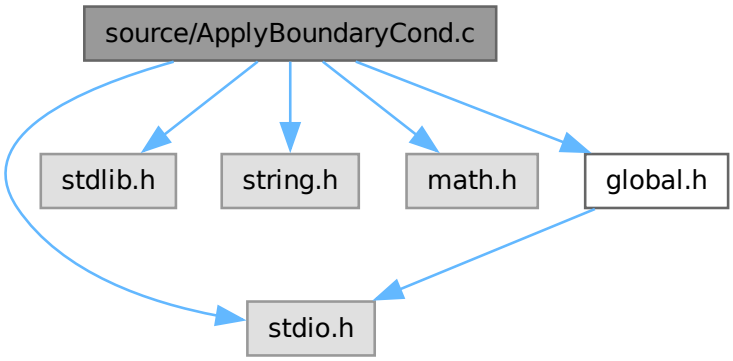
00017  Copyright (C) 2025 Harish Charan, University of Durham, UK
00018
00019  */
00020
00021 #include<stdio.h>
00022 #include<stdlib.h>
00023 #include"global.h"
00024
00025 void AllocArrays(){
00026  int n;
00027  // SPACETIME CORRELATIONS
00028  cfOrg = (double **) malloc ((nBuffCorr+1)*sizeof(double *));
00029  for (n = 0; n <= nBuffCorr; n++)
00030   cfOrg[n] = (double *) malloc ((2*nFunCorr+1)*sizeof(double));
00031
00032  cfVal = (double *) malloc ((2*nFunCorr+1)*sizeof(double));
00033  indexCorr = (int *) malloc ((nBuffCorr+1)*sizeof(int));
00034
00035  spacetimeCorr = (double **) malloc ((nBuffCorr+1)*sizeof(double));
00036  for (n = 0; n <= nBuffCorr; n++)
00037  spacetimeCorr[n] = (double *) malloc ((nFunCorr*nValCorr+1)*sizeof(double));
00038
00039  spacetimeCorrAv = (double *) malloc ((nFunCorr*nValCorr+1)*sizeof(double));
00040  // VISCOSITY
00041  indexAcf = (double *)malloc((nBuffAcf+1)*sizeof(double));
00042  viscAcf = (double **)malloc((nBuffAcf+1)*sizeof(double *));
00043  for(n = 0 ; n <= nBuffAcf ; n ++)
00044   viscAcf[n] = (double *)malloc((nValAcf+1)*sizeof(double ));
00045
00046  viscAcfOrg = (double *)malloc((nBuffAcf+1)*sizeof(double));
00047  viscAcfAv = (double *)malloc((nValAcf+1)*sizeof(double));
00048
00049   // RDF
00050   histRdf = (double *)malloc((sizeHistRdf+1)*sizeof(double));
00051 }
```

3.8 source/ApplyBoundaryCond.c File Reference

```
#include <stdio.h>
#include <stdlib.h>
#include <string.h>
#include <math.h>
#include "global.h"
```

Include dependency graph for ApplyBoundaryCond.c:



Functions

- void ApplyBoundaryCond ()

3.8.1 Function Documentation

3.8.1.1 ApplyBoundaryCond()

```
void ApplyBoundaryCond ( )
```

Definition at line 27 of file ApplyBoundaryCond.c.

```
00027                          {
00028   int n;
00029   for(n = 1 ; n <= nAtom ; n ++){
00030    if(strcmp(xBoundary, "p") == 0 && strcmp(yBoundary, "p") == 0){         // P.B.C along x and y axis
00031     rx[n] -= region[1]*rint(rx[n]/region[1]);
00032     ry[n] -= region[2]*rint(ry[n]/region[2]);
00033    } else if (strcmp(xBoundary, "r") == 0 && strcmp(yBoundary, "r") == 0){   //R.B.C. along x and y
      axis
00034      if((rx[n] + atomRadius[n]) >= regionH[1]){
00035         rx[n] = 0.999999*regionH[1] - atomRadius[n]; vx[n] = -vx[n] ;
00036      }if((rx[n]-atomRadius[n]) < -regionH[1]){
00037         rx[n] = -0.999999*regionH[1] + atomRadius[n]; vx[n] = -vx[n] ;
00038     }
00039      if((ry[n] + atomRadius[n])>= regionH[2]){
00040         ry[n] = 0.999999*regionH[2] - atomRadius[n]; vy[n] = -vy[n] ;
00041      }if((ry[n]-atomRadius[n]) < -regionH[2]){
00042         ry[n] = -0.999999*regionH[2] + atomRadius[n]; vy[n] = -vy[n] ;
00043     }}
00044     else if (strcmp(xBoundary, "p") == 0 && strcmp(yBoundary, "r") == 0){   //P.B.C. along x and R.B.C
      along y axis
00045     rx[n] -= region[1]*rint(rx[n]/region[1]);
00046     if((ry[n] + atomRadius[n]) >= regionH[2]){
00047       ry[n] = 0.999999*regionH[2] - atomRadius[n]; vy[n] = -vy[n] ;
00048      }if((ry[n] - atomRadius[n]) < -regionH[2]){
00049         ry[n] = -0.999999*regionH[2] + atomRadius[n]; vy[n] = -vy[n] ;
00050   }}
00051     else if(strcmp(xBoundary, "r") == 0 && strcmp(yBoundary, "p") == 0){   //R.B.C. along x and P.B.C
      along y axis
00052     if((rx[n] + atomRadius[n]) >= regionH[1]){
00053        rx[n] = 0.999999*regionH[1] - atomRadius[n]; vx[n] = -vx[n] ;
00054      }if((rx[n] - atomRadius[n]) < -regionH[1]){
00055       rx[n] = -0.999999*regionH[1] + atomRadius[n]; vx[n] = -vx[n] ;
00056      }
00057      ry[n] -= region[2]*rint(ry[n]/region[2]);
00058   } else {
00059     // Print error message and exit the program
00060     fprintf(fpresult, "Error: Invalid boundary configuration: '%s %s'\n", xBoundary, yBoundary);
00061     exit(EXIT_FAILURE); // Exit with failure status
00062   }
00063  }
00064 }
```

References atomRadius, fpresult, nAtom, region, regionH, rx, ry, vx, vy, xBoundary, and yBoundary.

Referenced by main().

Here is the caller graph for this function:

3.9 ApplyBoundaryCond.c

Go to the documentation of this file.

```
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00012  * GNU General Public License for more details.
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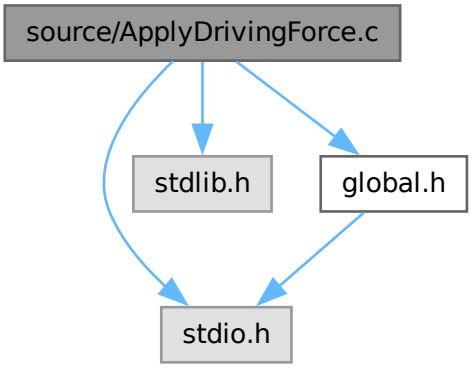
00015  * along with Lamina. If not, see <https://www.gnu.org/licenses/>.
00016
00017  Copyright (C) 2025 Harish Charan, University of Durham, UK
00018
00019  */
00020
00021 #include<stdio.h>
00022 #include<stdlib.h>
00023 #include<string.h>
00024 #include<math.h>
00025 #include"global.h"
00026
00027 void ApplyBoundaryCond(){
00028   int n;
00029   for(n = 1 ; n <= nAtom ; n ++){
00030    if(strcmp(xBoundary, "p") == 0 && strcmp(yBoundary, "p") == 0){         // P.B.C along x and y axis
00031     rx[n] -= region[1]*rint(rx[n]/region[1]);
00032     ry[n] -= region[2]*rint(ry[n]/region[2]);
00033    } else if (strcmp(xBoundary, "r") == 0 && strcmp(yBoundary, "r") == 0){   //R.B.C. along x and y
      axis
00034      if((rx[n] + atomRadius[n]) >= regionH[1]){
00035         rx[n] = 0.999999*regionH[1] - atomRadius[n]; vx[n] = -vx[n] ;
00036      }if((rx[n]-atomRadius[n]) < -regionH[1]){
00037         rx[n] = -0.999999*regionH[1] + atomRadius[n]; vx[n] = -vx[n] ;
00038     }
00039      if((ry[n] + atomRadius[n])>= regionH[2]){
00040         ry[n] = 0.999999*regionH[2] - atomRadius[n]; vy[n] = -vy[n] ;
00041      }if((ry[n]-atomRadius[n]) < -regionH[2]){
00042         ry[n] = -0.999999*regionH[2] + atomRadius[n]; vy[n] = -vy[n] ;
00043     }}
00044     else if (strcmp(xBoundary, "p") == 0 && strcmp(yBoundary, "r") == 0){   //P.B.C. along x and R.B.C
      along y axis
00045     rx[n] -= region[1]*rint(rx[n]/region[1]);
00046     if((ry[n] + atomRadius[n]) >= regionH[2]){
00047       ry[n] = 0.999999*regionH[2] - atomRadius[n]; vy[n] = -vy[n] ;
00048      }if((ry[n] - atomRadius[n]) < -regionH[2]){
00049         ry[n] = -0.999999*regionH[2] + atomRadius[n]; vy[n] = -vy[n] ;
00050   }}
00051     else if(strcmp(xBoundary, "r") == 0 && strcmp(yBoundary, "p") == 0){   //R.B.C. along x and P.B.C
      along y axis
00052     if((rx[n] + atomRadius[n]) >= regionH[1]){
00053        rx[n] = 0.999999*regionH[1] - atomRadius[n]; vx[n] = -vx[n] ;
00054      }if((rx[n] - atomRadius[n]) < -regionH[1]){
00055       rx[n] = -0.999999*regionH[1] + atomRadius[n]; vx[n] = -vx[n] ;
00056      }
00057      ry[n] -= region[2]*rint(ry[n]/region[2]);
00058   } else {
00059     // Print error message and exit the program
00060     fprintf(fpresult, "Error: Invalid boundary configuration: '%s %s'\n", xBoundary, yBoundary);
00061     exit(EXIT_FAILURE); // Exit with failure status
00062   }
00063  }
00064 }
```

3.10 source/ApplyDrivingForce.c File Reference

```
#include <stdio.h>
#include <stdlib.h>
```

```
#include "global.h"
```

Include dependency graph for ApplyDrivingForce.c:



Functions

- void ApplyDrivingForce ()

3.10.1 Function Documentation

3.10.1.1 ApplyDrivingForce()

```
void ApplyDrivingForce ( )
```

Definition at line 25 of file ApplyDrivingForce.c.

```
00025                           {
00026  int n;
00027  double Vxblock, Vyblock;
00028  double Vxsubstrate, Vysubstrate;
00029  Vxblock = 0.0;  Vyblock = 0.0;
00030  Vxsubstrate = 0.0; Vysubstrate = 0.0;
00031  double gammav;
00032  gammav = 0.0;
00033
00034  double count_substrate = 0;
00035  double count_block = 0;
00036
00037  for(n = 1 ; n <= nAtom; n ++){
00038   if(atomType[n] == 1 || atomType[n] == 2){
00039   Vxsubstrate += vx[n]; Vysubstrate += vy[n];
00040   count_substrate++;
00041   }
00042   if(atomType[n] == 3 || atomType[n] == 4){
00043   Vxblock += vx[n]; Vyblock += vy[n];
00044   count_block++;
00045   } }
00046
00047   if(count_substrate > 0) {
00048     Vxsubstrate /= count_substrate;
00049     Vysubstrate /= count_substrate;
00050   }
00051
00052   if(count_block > 0) {
00053    Vxblock /= count_block;
00054    Vyblock /= count_block;
00055   }
```

```
00056
00057  for(n = 1 ; n <= nAtom; n ++){
00058   if(atomType[n] == 1 || atomType[n] == 2){
00059   ax[n] += -gammav * (vx[n] - Vxsubstrate);
00060   ay[n] += -gammav * (vy[n] - Vysubstrate);
00061   }
00062   if(atomType[n] == 3 || atomType[n] == 4){
00063   ax[n] += -gammav * (vx[n] - Vxblock);
00064   ay[n] += -gammav * (vy[n] - Vyblock);
00065  } } }
```

References atomType, ax, ay, nAtom, vx, and vy.

3.11 ApplyDrivingForce.c

Go to the documentation of this file.

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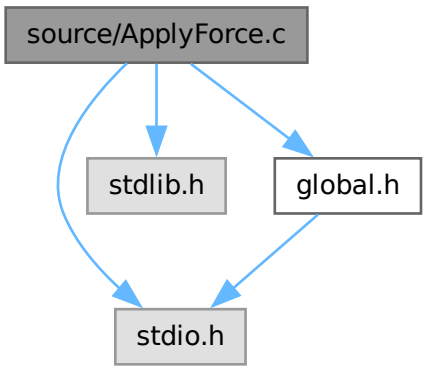
00016
00017  Copyright (C) 2025 Harish Charan, University of Durham, UK
00018
00019  */
00020
00021 #include<stdio.h>
00022 #include<stdlib.h>
00023 #include"global.h"
00024
00025 void ApplyDrivingForce(){
00026  int n;
00027  double Vxblock, Vyblock;
00028  double Vxsubstrate, Vysubstrate;
00029  Vxblock = 0.0;  Vyblock = 0.0;
00030  Vxsubstrate = 0.0; Vysubstrate = 0.0;
00031  double gammav;
00032  gammav = 0.0;
00033
00034  double count_substrate = 0;
00035  double count_block = 0;
00036
00037  for(n = 1 ; n <= nAtom; n ++){
00038   if(atomType[n] == 1 || atomType[n] == 2){
00039   Vxsubstrate += vx[n]; Vysubstrate += vy[n];
00040   count_substrate++;
00041   }
00042   if(atomType[n] == 3 || atomType[n] == 4){
00043   Vxblock += vx[n]; Vyblock += vy[n];
00044   count_block++;
00045   } }
00046
00047   if(count_substrate > 0) {
00048     Vxsubstrate /= count_substrate;
00049     Vysubstrate /= count_substrate;
00050   }
00051
00052   if(count_block > 0) {
00053    Vxblock /= count_block;
00054    Vyblock /= count_block;
00055   }
00056
00057  for(n = 1 ; n <= nAtom; n ++){
00058   if(atomType[n] == 1 || atomType[n] == 2){
00059   ax[n] += -gammav * (vx[n] - Vxsubstrate);
00060   ay[n] += -gammav * (vy[n] - Vysubstrate);
00061   }
00062   if(atomType[n] == 3 || atomType[n] == 4){
00063   ax[n] += -gammav * (vx[n] - Vxblock);
00064   ay[n] += -gammav * (vy[n] - Vyblock);
00065  } } }
00066
00067
```

3.12 source/ApplyForce.c File Reference

```
#include <stdio.h>
#include <stdlib.h>
#include "global.h"
```

Include dependency graph for ApplyForce.c:



Functions

- void ApplyForce ()

3.12.1 Function Documentation

3.12.1.1 ApplyForce()

```
void ApplyForce ( )
```

Definition at line 25 of file ApplyForce.c.

```
00025                   {
00026  int n;
00027  double lx;
00028  lx = regionH[1];
00029  fy =  (FyBylx * lx)/nAtomBlock;
00030  fx =  fxByfy * fy;
00031  for(n = 1; n <= nAtom; n ++){
00032  if(molID[n] == 2){
00033   ax[n] += fx;
00034   ay[n] -= fy;
00035 } } }
```

References ax, ay, fx, fxByfy, fy, FyBylx, molID, nAtom, nAtomBlock, and regionH.

Referenced by main().

Here is the caller graph for this function:

3.13 ApplyForce.c

Go to the documentation of this file.

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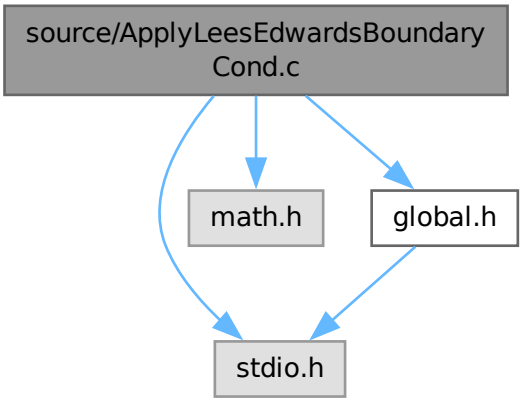
00016
00017  Copyright (C) 2025 Harish Charan, University of Durham, UK
00018
00019  */
00020
00021 #include<stdio.h>
00022 #include<stdlib.h>
00023 #include"global.h"
00024
00025 void ApplyForce(){
00026  int n;
00027  double lx;
00028  lx = regionH[1];
00029  fy =  (FyBylx * lx)/nAtomBlock;
00030  fx =  fxByfy * fy;
00031  for(n = 1; n <= nAtom; n ++){
00032  if(molID[n] == 2){
00033   ax[n] += fx;
00034   ay[n] -= fy;
00035 } } }
```

3.14 source/ApplyLeesEdwardsBoundaryCond.c File Reference

```
#include <stdio.h>
#include <math.h>
#include "global.h"
```

Include dependency graph for ApplyLeesEdwardsBoundaryCond.c:



Functions

- void ApplyLeesEdwardsBoundaryCond ()

3.14.1 Function Documentation

3.14.1.1 ApplyLeesEdwardsBoundaryCond()

```
void ApplyLeesEdwardsBoundaryCond ( )
```

Definition at line 25 of file ApplyLeesEdwardsBoundaryCond.c.

```
00025                                  {
00026  int n;
00027  for (n = 1; n <= nAtom; n++) {
00028 //PBC along x-direction
00029  if(rx[n] >= regionH[1])
00030    rx[n] -= region[1];
00031  else if(rx[n] < -regionH[1])
00032    rx[n] += region[1];
00033
00034 //LEBC along y-direction
00035   if(ry[n] >= regionH[2]){
00036    rx[n] -= shearDisplacement;
00037    if(rx[n] < -regionH[1]) rx[n] += region[1];
00038    //vx[n] -= shearVelocity;
00039    ry[n] -= region[2];
00040   }else if(ry[n] < -regionH[2]){
00041    rx[n] += shearDisplacement;
00042    if(rx[n] >= regionH[1]) rx[n] -= region[1];
00043    //vx[n] += shearVelocity;
00044    ry[n] += region[2];
00045   }
00046  }
00047 }
```

References nAtom, region, regionH, rx, ry, and shearDisplacement.

3.15 ApplyLeesEdwardsBoundaryCond.c

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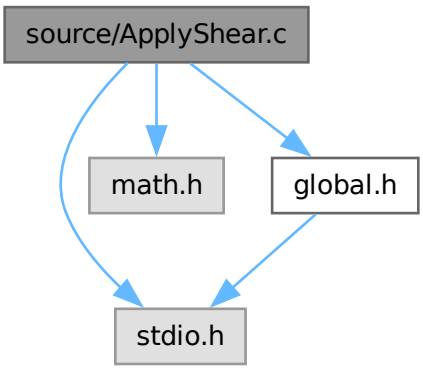
00016
00017  Copyright (C) 2025 Harish Charan, University of Durham, UK
00018
00019  */
00020
00021 #include <stdio.h>
00022 #include <math.h>
00023 #include "global.h"
00024
00025 void ApplyLeesEdwardsBoundaryCond() {
00026  int n;
00027  for (n = 1; n <= nAtom; n++) {
00028 //PBC along x-direction
00029  if(rx[n] >= regionH[1])
00030    rx[n] -= region[1];
00031  else if(rx[n] < -regionH[1])
00032    rx[n] += region[1];
00033
00034 //LEBC along y-direction
00035   if(ry[n] >= regionH[2]){
00036    rx[n] -= shearDisplacement;
00037    if(rx[n] < -regionH[1]) rx[n] += region[1];
00038    //vx[n] -= shearVelocity;
00039    ry[n] -= region[2];
00040   }else if(ry[n] < -regionH[2]){
00041    rx[n] += shearDisplacement;
00042    if(rx[n] >= regionH[1]) rx[n] -= region[1];
00043    //vx[n] += shearVelocity;
00044    ry[n] += region[2];
00045   }
00046  }
00047 }
00048
```

3.16 source/ApplyShear.c File Reference

```
#include <stdio.h>
#include <math.h>
#include "global.h"
```

Include dependency graph for ApplyShear.c:



Functions

- void ApplyShear ()

3.16.1 Function Documentation

3.16.1.1 ApplyShear()

```
void ApplyShear ( )
```

Definition at line 25 of file ApplyShear.c.

```
00025                   {
00026  int n;
00027  for(n = 1 ; n <= nAtom ; n ++){
00028   rx[n] += strain * ry[n];
00029   //vx[n] += stranRate * ry[n];
00030  } }
```

References nAtom, rx, ry, and strain.

3.17 ApplyShear.c

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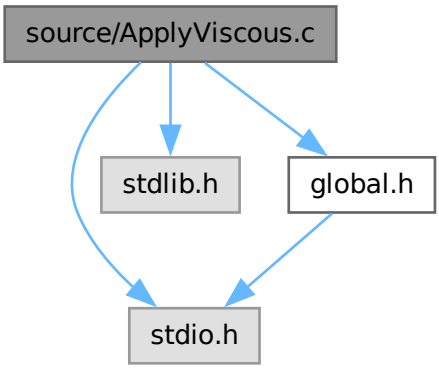
00018
00019  */
00020
00021 #include<stdio.h>
00022 #include<math.h>
00023 #include"global.h"
00024
00025 void ApplyShear(){
00026  int n;
00027  for(n = 1 ; n <= nAtom ; n ++){
00028   rx[n] += strain * ry[n];
00029   //vx[n] += stranRate * ry[n];
00030  } }
```

3.18 source/ApplyViscous.c File Reference

```
#include <stdio.h>
#include <stdlib.h>
#include "global.h"
```

Include dependency graph for ApplyViscous.c:



Functions

- void ApplyViscous ()

3.18.1 Function Documentation

3.18.1.1 ApplyViscous()

```
void ApplyViscous ( )
```

Definition at line 25 of file ApplyViscous.c.

```
00025                    {
00026  int n;
00027  double gammav;
00028  gammav = 1.0;
00029  for(n = 1 ; n <= nAtom; n ++){
00030   ax[n] += -gammav * vx[n];
00031   ay[n] += -gammav * vy[n];
00032  } }
```

References ax, ay, nAtom, vx, and vy.

3.19 ApplyViscous.c

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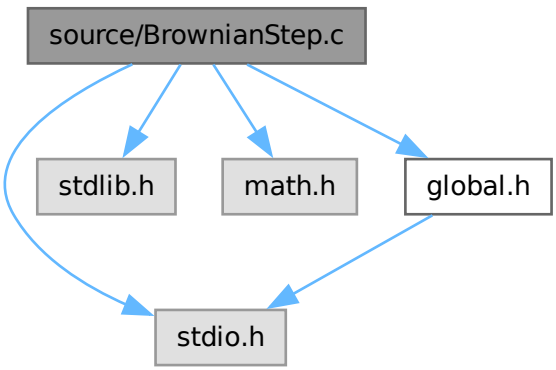
00017  Copyright (C) 2025 Harish Charan, University of Durham, UK
00018
00019  */
00020
00021 #include<stdio.h>
00022 #include<stdlib.h>
00023 #include"global.h"
00024
00025 void ApplyViscous(){
00026  int n;
00027  double gammav;
00028  gammav = 1.0;
00029  for(n = 1 ; n <= nAtom; n ++){
00030   ax[n] += -gammav * vx[n];
00031   ay[n] += -gammav * vy[n];
00032  } }
00033
00034
```

3.20 source/BrownianStep.c File Reference

```
#include <stdio.h>
#include <stdlib.h>
#include <math.h>
#include "global.h"
```

Include dependency graph for BrownianStep.c:



Functions

- void BrownianStep ()

3.20.1 Function Documentation

3.20.1.1 BrownianStep()

```
void BrownianStep ( )
```

Definition at line 26 of file BrownianStep.c.

```
00026                    {
00027   if(stepCount <= stepEquil){
00028     double A, S1, S2, T;
00029     int n;
00030     S1 = 0.; S2 = 0;
00031     double halfdt = 0.5*deltaT;
00032     for (n = 1; n <= nAtom; n++){
00033       T = vx[n] + halfdt * ax[n];
00034       S1 += T * ax[n];
00035       S2 += Sqr(T);
00036 
00037       T = vy[n] + halfdt * ay[n];
00038       S1 += T * ay[n];
00039       S2 += Sqr(T);
00040     }
00041     A = -S1 / S2;
00042     double C = 1 + A*deltaT ;
00043     double D = deltaT * (1 + 0.5 * A * deltaT);
00044     for (n = 1; n <= nAtom; n++){
00045       vx[n] = C * vx[n] + D * ax[n];
00046       rx[n] += deltaT * vx[n];
00047       vy[n] = C * vy[n] + D * ay[n];
00048       ry[n] += deltaT * vy[n];
00049     }
00050   }else{
00051       int n;
00052       //SETTING TEMP = 0.0
00053      if (stepCount == stepEquil+1){
00054      for(n = 1 ; n <= nAtom ; n ++){
00055      vx[n] = 0.0;
00056      vy[n] = 0.0;
00057      }}
00058      double zeta = 1.0;
00059      double dx, dy;
00060      for(n = 1 ; n <= nAtom ; n ++){
00061       dx = rx[n];
00062       rx[n] += zeta * ax[n] * deltaT;
00063       dx = rx[n] - dx;
00064       vx[n] = dx/deltaT;
00065       dy = ry[n];
00066       ry[n] += zeta * ay[n] * deltaT;
00067       dy = ry[n] - dy;
00068       vy[n] = dy/deltaT;
00069     }
00070   }
00071 }
```

References ax, ay, deltaT, nAtom, rx, ry, Sqr, stepCount, stepEquil, vx, and vy.

3.21 BrownianStep.c

Go to the documentation of this file.

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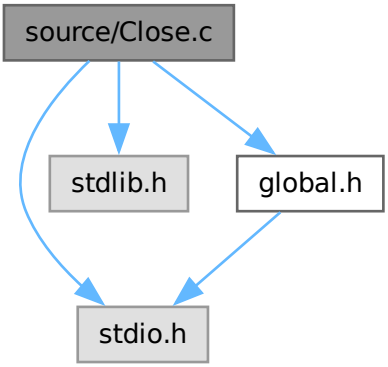
00017  Copyright (C) 2025 Harish Charan, University of Durham, UK
00018
00019  */
00020
00021 #include<stdio.h>
00022 #include<stdlib.h>
00023 #include<math.h>
00024 #include"global.h"
00025
00026 void BrownianStep(){
00027   if(stepCount <= stepEquil){
00028     double A, S1, S2, T;
00029     int n;
00030     S1 = 0.; S2 = 0;
00031     double halfdt = 0.5*deltaT;
00032     for (n = 1; n <= nAtom; n++){
00033       T = vx[n] + halfdt * ax[n];
00034       S1 += T * ax[n];
00035       S2 += Sqr(T);
00036
00037       T = vy[n] + halfdt * ay[n];
00038       S1 += T * ay[n];
00039       S2 += Sqr(T);
00040     }
00041     A = -S1 / S2;
00042     double C = 1 + A*deltaT ;
00043     double D = deltaT * (1 + 0.5 * A * deltaT);
00044     for (n = 1; n <= nAtom; n++){
00045       vx[n] = C * vx[n] + D * ax[n];
00046       rx[n] += deltaT * vx[n];
00047       vy[n] = C * vy[n] + D * ay[n];
00048       ry[n] += deltaT * vy[n];
00049     }
00050   }else{
00051       int n;
00052       //SETTING TEMP = 0.0
00053      if (stepCount == stepEquil+1){
00054      for(n = 1 ; n <= nAtom ; n ++){
00055      vx[n] = 0.0;
00056      vy[n] = 0.0;
00057      }}
00058      double zeta = 1.0;
00059      double dx, dy;
00060      for(n = 1 ; n <= nAtom ; n ++){
00061       dx = rx[n];
00062       rx[n] += zeta * ax[n] * deltaT;
00063       dx = rx[n] - dx;
00064       vx[n] = dx/deltaT;
00065       dy = ry[n];
00066       ry[n] += zeta * ay[n] * deltaT;
00067       dy = ry[n] - dy;
00068       vy[n] = dy/deltaT;
00069     }
00070   }
00071 }
00072
```

3.22 source/Close.c File Reference

```
#include <stdio.h>
#include <stdlib.h>
#include "global.h"
```

Include dependency graph for Close.c:



Functions

- void Close ()

3.22.1 Function Documentation

3.22.1.1 Close()

```
void Close ( )
```

Definition at line 24 of file Close.c.

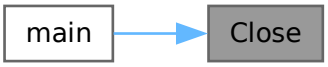
```
00024           {
00025   int n;
00026   free(rx);
00027   free(ry);
00028   free(vx);
00029   free(vy);
00030   free(ax);
00031   free(ay);
00032   free(fax);
00033   free(fay);
00034   free(cellList);
00035
00036   free(atomID); free(atomType); free(atomRadius); free(atomMass);
00037   free(speed);
00038   free(atom1); free(atom2); free(BondID);
00039   free(BondType); free(kb); free(ro);
00040   free(ImageX); free(ImageY); free(rxUnwrap); free(ryUnwrap);
00041   free(atomIDInterface);
00042   free(PairID); free(Pairatom1); free(Pairatom2);
00043   free(PairXij); free(PairYij);
00044
00045   free(DeltaXijOld);
00046   free(DeltaYijOld);
00047
00048   free(molID);
00049
00050   for (n = 0; n <= nAtom; n++) {
00051    free(isBonded[n]);
00052    }
00053    free(isBonded);
00054
00055
00056
```

```
00057   for(n = 0; n <= nAtom; n++) {
00058    free(DeltaXijOldPair[n]);
00059    free(DeltaYijOldPair[n]);
00060    }
00061     free(DeltaXijOldPair);
00062     free(DeltaYijOldPair);
00063
00064   for (n = 0; n <= nBuffCorr; n++){
00065     free(cfOrg[n]);
00066     free(spacetimeCorr[n]);
00067   }
00068   free(cfOrg);
00069   free(spacetimeCorr);
00070   free(cfVal);
00071   free(indexCorr);
00072   free(spacetimeCorrAv);
00073
00074   free(indexAcf);
00075   free(viscAcfOrg);
00076   free(viscAcfAv);
00077   for(n = 0 ; n <= nBuffAcf ; n ++)
00078     free(viscAcf[n]);
00079   free(viscAcf);
00080
00081 }
```

References atom1, atom2, atomID, atomIDInterface, atomMass, atomRadius, atomType, ax, ay, BondID, BondType, cellList, cfOrg, cfVal, DeltaXijOld, DeltaXijOldPair, DeltaYijOld, DeltaYijOldPair, fax, fay, ImageX, ImageY, indexAcf, indexCorr, isBonded, kb, molID, nAtom, nBuffAcf, nBuffCorr, Pairatom1, Pairatom2, PairID, PairXij, PairYij, ro, rx, rxUnwrap, ry, ryUnwrap, spacetimeCorr, spacetimeCorrAv, speed, viscAcf, viscAcfAv, viscAcfOrg, vx, and vy.

Referenced by main().

Here is the caller graph for this function:



3.23 Close.c

Go to the documentation of this file.

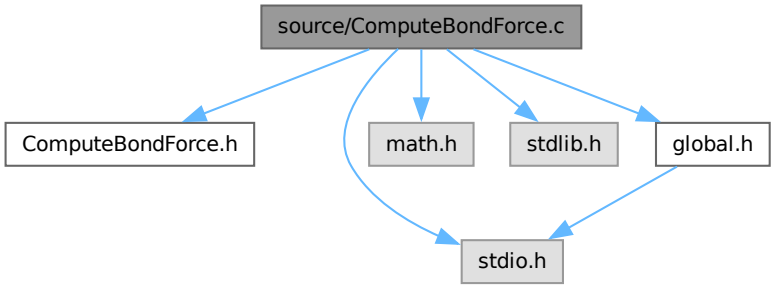
```
00001 /*
00002  * This file is part of Lamina.
00003  *
00004  * Lamina is free software: you can redistribute it and/or modify
00005  * it under the terms of the GNU General Public License as published by
00006  * the Free Software Foundation, either version 3 of the License, or
00007  * (at your option) any later version.
00008  *
00009  * Lamina is distributed in the hope that it will be useful,
00010  * but WITHOUT ANY WARRANTY; without even the implied warranty of
00011  * MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the
00012  * GNU General Public License for more details.
00013  *
00014  * You should have received a copy of the GNU General Public License
00015  * along with Lamina. If not, see <https://www.gnu.org/licenses/>.
00016
00017  Copyright (C) 2025 Harish Charan, University of Durham, UK
00018
00019  */
00020
00021 #include<stdio.h>
00022 #include<stdlib.h>
```

```
00023 #include"global.h"
00024 void Close(){
00025   int n;
00026   free(rx);
00027   free(ry);
00028   free(vx);
00029   free(vy);
00030   free(ax);
00031   free(ay);
00032   free(fax);
00033   free(fay);
00034   free(cellList);
00035
00036   free(atomID); free(atomType); free(atomRadius); free(atomMass);
00037   free(speed);
00038   free(atom1); free(atom2); free(BondID);
00039   free(BondType); free(kb); free(ro);
00040   free(ImageX); free(ImageY); free(rxUnwrap); free(ryUnwrap);
00041   free(atomIDInterface);
00042   free(PairID); free(Pairatom1); free(Pairatom2);
00043   free(PairXij); free(PairYij);
00044
00045   free(DeltaXijOld);
00046   free(DeltaYijOld);
00047
00048   free(molID);
00049
00050   for (n = 0; n <= nAtom; n++) {
00051    free(isBonded[n]);
00052    }
00053    free(isBonded);
00054
00055
00056
00057   for(n = 0; n <= nAtom; n++) {
00058    free(DeltaXijOldPair[n]);
00059    free(DeltaYijOldPair[n]);
00060    }
00061     free(DeltaXijOldPair);
00062     free(DeltaYijOldPair);
00063
00064   for (n = 0; n <= nBuffCorr; n++){
00065     free(cfOrg[n]);
00066     free(spacetimeCorr[n]);
00067   }
00068   free(cfOrg);
00069   free(spacetimeCorr);
00070   free(cfVal);
00071   free(indexCorr);
00072   free(spacetimeCorrAv);
00073
00074   free(indexAcf);
00075   free(viscAcfOrg);
00076   free(viscAcfAv);
00077   for(n = 0 ; n <= nBuffAcf ; n ++)
00078     free(viscAcf[n]);
00079   free(viscAcf);
00080
00081 }
```

3.24 source/ComputeBondForce.c File Reference

```
#include "ComputeBondForce.h"
#include <stdio.h>
#include <math.h>
#include <stdlib.h>
#include "global.h"
```

Include dependency graph for ComputeBondForce.c:



Functions

- void ComputeBondForce ()

3.24.1 Function Documentation

3.24.1.1 ComputeBondForce()

```
void ComputeBondForce ( )
```

Definition at line 28 of file ComputeBondForce.c.

```
00028                           {
00029   int n;
00030   double dr[NDIM+1], r, rr, ri, roi;
00031   double uVal, fcVal;
00032
00033   uVal = 0.0; TotalBondEnergy = 0.0;
00034   virSumBond = 0.0; virSumBondxx = 0.0; virSumBondyy = 0.0; virSumBondxy = 0.0;
00035
00036   double vr[NDIM+1], fdVal, rri;
00037
00038   for(n = 1 ; n <= nAtom ; n ++){
00039    nodeDragx[n] = 0.0;
00040    nodeDragy[n] = 0.0;
00041   } //Important change made on 03Apr2025. Mention it in GitHub
00042
00043   int atom1ID, atom2ID;
00044
00045   for(n=1; n<=nBond; n++){
00046    rr = 0.0; rri = 0.0; fcVal = 0.0;  fdVal = 0.0; strech = 0.0;
00047    atom1ID = atom1[n];
00048    atom2ID = atom2[n];
00049
00050    dr[1] = rx[atom1ID] - rx[atom2ID];
00051    if(dr[1] >= regionH[1])
00052     dr[1] -= region[1];
00053    else if(dr[1] < -regionH[1])
00054     dr[1] += region[1];
00055
00056    dr[2] = ry[atom1ID] - ry[atom2ID];
00057    if(dr[2] >= regionH[2]){
00058     dr[1] -= shearDisplacement;
00059     if(dr[1] < -regionH[1]) dr[1] += region[1];
00060     dr[2] -= region[2];
00061   }else if(dr[2] < -regionH[2]){
00062    dr[1] += shearDisplacement;
00063     if(dr[1] >= regionH[1]) dr[1] -= region[1];
00064    dr[2] += region[2];
00065   }
00066
```

```
00067    rr = Sqr(dr[1]) + Sqr(dr[2]);
00068    r = sqrt(rr);
00069    rri = 1.0/rr;
00070    ri = 1.0/r;
00071    roi = 1.0/ro[n];
00072    strech = (r * roi - 1.0);
00073    uVal = 0.5 * kb[n] * ro[n] * Sqr(strech);
00074    fcVal = -kb[n] * strech * ri; //F = -Grad U
00075
00076    vr[1] = vx[atom1ID] - vx[atom2ID];
00077    vr[2] = vy[atom1ID] - vy[atom2ID];
00078    fdVal = -gamman * (vr[1]*dr[1] + vr[2]*dr[2]) * rri; //node-node drag
00079
00080    //DampFlag = 1. LAMMPS version
00081    if(DampFlag == 1){
00082    nodeDragx[atom1ID] =  fdVal * dr[1];  //node-node drag  //Important change made on 03Apr2025.
     Mention it in GitHub
00083    nodeDragy[atom1ID] =  fdVal * dr[2];  //node-node drag  //Adding the drag forces is wrong. Only add
     the
00084    nodeDragx[atom2ID] =  -fdVal * dr[1];  //node-node drag //total force
00085    nodeDragy[atom2ID] =  -fdVal * dr[2];  //node-node drag
00086
00087    ax[atom1ID] +=  (fcVal + fdVal) * dr[1];
00088    ay[atom1ID] +=  (fcVal + fdVal) * dr[2];
00089    ax[atom2ID] += -(fcVal + fdVal) * dr[1];
00090    ay[atom2ID] += -(fcVal + fdVal) * dr[2];
00091    }
00092
00093    //DampFlag = 2. Suzanne notes version
00094    else if(DampFlag == 2){
00095    nodeDragx[atom1ID] =  -gamman * vr[1];  //node-node drag
00096    nodeDragy[atom1ID] =  -gamman * vr[2]; //node-node drag
00097    nodeDragx[atom2ID] =  -(-gamman * vr[1]);  //node-node drag
00098    nodeDragy[atom2ID] =  -(-gamman * vr[2]);  //node-node drag
00099
00100    ax[atom1ID] +=  (fcVal * dr[1] - gamman * vr[1]);
00101    ay[atom1ID] +=  (fcVal * dr[2] - gamman * vr[2]);
00102    ax[atom2ID] += -(fcVal * dr[1] - gamman * vr[1]);
00103    ay[atom2ID] += -(fcVal * dr[2] - gamman * vr[2]);
00104    }
00105
00106    //DampFlag = 3. Suzanne PRL, 130, 178203 (2023) version
00107    else if(DampFlag == 3){
00108     DeltaXijNew = dr[1];
00109     DeltaYijNew = dr[2];
00110
00111     if(stepCount == 0) {  // First timestep
00112      DeltaXijOld[n] = DeltaXijNew;
00113      DeltaYijOld[n] = DeltaYijNew;
00114     }
00115
00116     DeltaXij = DeltaXijNew - DeltaXijOld[n];
00117     DeltaYij = DeltaYijNew - DeltaYijOld[n];
00118     DeltaVXij = DeltaXij / deltaT;
00119     DeltaVYij = DeltaYij / deltaT;
00120
00121     // Now update for the next timestep
00122     DeltaXijOld[n] = DeltaXijNew;
00123     DeltaYijOld[n] = DeltaYijNew;
00124
00125     nodeDragx[atom1ID] =  -gamman * DeltaVXij;  //node-node drag
00126     nodeDragy[atom1ID] =  -gamman * DeltaVYij; //node-node drag
00127     nodeDragx[atom2ID] =  -(-gamman * DeltaVXij);  //node-node drag
00128     nodeDragy[atom2ID] =  -(-gamman * DeltaVYij);  //node-node drag
00129
00130     ax[atom1ID] +=  (fcVal * dr[1] - gamman * DeltaVXij);
00131     ay[atom1ID] +=  (fcVal * dr[2] - gamman * DeltaVYij);
00132     ax[atom2ID] += -(fcVal * dr[1] - gamman * DeltaVXij);
00133     ay[atom2ID] += -(fcVal * dr[2] - gamman * DeltaVYij);
00134    }
00135
00136
00137    BondLength[n] = r;
00138    BondEnergy[n] = uVal; //No 0.5 factor since it is the energy of the bond
00139    TotalBondEnergy   +=  BondEnergy[n];
00140
00141    virSumBond +=   0.5 * (fcVal + fdVal) * rr;
00142    virSumBondxx += 0.5 * (fcVal + fdVal) * dr[1] * dr[1];
00143    virSumBondyy += 0.5 * (fcVal + fdVal) * dr[2] * dr[2];
00144    virSumBondxy += 0.5 * (fcVal + fdVal) * dr[1] * dr[2];
00145 } }
```

References atom1, atom2, ax, ay, BondEnergy, BondLength, DampFlag, deltaT, DeltaVXij, DeltaVYij, DeltaXij, DeltaXijNew, DeltaXijOld, DeltaYij, DeltaYijNew, DeltaYijOld, gamman, kb, nAtom, nBond, NDIM, nodeDragx, nodeDragy, region, regionH, ro, rx, ry, shearDisplacement, Sqr, stepCount, strech, TotalBondEnergy, virSumBond, virSumBondxx, virSumBondxy, virSumBondyy, vx, and vy.

Referenced by main().

Here is the caller graph for this function:

3.25 ComputeBondForce.c

Go to the documentation of this file.

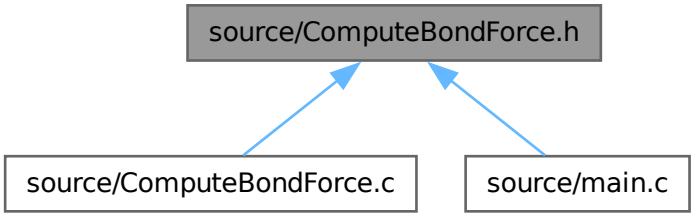
```
00001 /*
00002  * This file is part of Lamina.
00003  *
00004  * Lamina is free software: you can redistribute it and/or modify
00005  * it under the terms of the GNU General Public License as published by
00006  * the Free Software Foundation, either version 3 of the License, or
00007  * (at your option) any later version.
00008  *
00009  * Lamina is distributed in the hope that it will be useful,
00010  * but WITHOUT ANY WARRANTY; without even the implied warranty of
00011  * MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the
00012  * GNU General Public License for more details.
00013  *
00014  * You should have received a copy of the GNU General Public License
00015  * along with Lamina. If not, see <https://www.gnu.org/licenses/>.
00016
00017  Copyright (C) 2025 Harish Charan, University of Durham, UK
00018
00019  */
00020
00021 #include "ComputeBondForce.h"
00022
00023 #include<stdio.h>
00024 #include<math.h>
00025 #include<stdlib.h>
00026 #include"global.h"
00027
00028 void ComputeBondForce(){
00029   int n;
00030   double dr[NDIM+1], r, rr, ri, roi;
00031   double uVal, fcVal;
00032
00033   uVal = 0.0; TotalBondEnergy = 0.0;
00034   virSumBond = 0.0; virSumBondxx = 0.0; virSumBondyy = 0.0; virSumBondxy = 0.0;
00035
00036   double vr[NDIM+1], fdVal, rri;
00037
00038   for(n = 1 ; n <= nAtom ; n ++){
00039    nodeDragx[n] = 0.0;
00040    nodeDragy[n] = 0.0;
00041   } //Important change made on 03Apr2025. Mention it in GitHub
00042
00043   int atom1ID, atom2ID;
00044
00045   for(n=1; n<=nBond; n++){
00046    rr = 0.0; rri = 0.0; fcVal = 0.0;  fdVal = 0.0; strech = 0.0;
00047    atom1ID = atom1[n];
00048    atom2ID = atom2[n];
00049
00050    dr[1] = rx[atom1ID] - rx[atom2ID];
00051    if(dr[1] >= regionH[1])
00052     dr[1] -= region[1];
00053    else if(dr[1] < -regionH[1])
00054     dr[1] += region[1];
00055
00056    dr[2] = ry[atom1ID] - ry[atom2ID];
00057    if(dr[2] >= regionH[2]){
```

```
00058     dr[1] -= shearDisplacement;
00059     if(dr[1] < -regionH[1]) dr[1] += region[1];
00060     dr[2] -= region[2];
00061    }else if(dr[2] < -regionH[2]){
00062     dr[1] += shearDisplacement;
00063     if(dr[1] >= regionH[1]) dr[1] -= region[1];
00064     dr[2] += region[2];
00065    }
00066
00067     rr = Sqr(dr[1]) + Sqr(dr[2]);
00068     r = sqrt(rr);
00069     rri = 1.0/rr;
00070     ri = 1.0/r;
00071     roi = 1.0/ro[n];
00072     strech = (r * roi - 1.0);
00073     uVal = 0.5 * kb[n] * ro[n] * Sqr(strech);
00074     fcVal = -kb[n] * strech * ri; //F = -Grad U
00075
00076     vr[1] = vx[atom1ID] - vx[atom2ID];
00077     vr[2] = vy[atom1ID] - vy[atom2ID];
00078     fdVal = -gamman * (vr[1]*dr[1] + vr[2]*dr[2]) * rri; //node-node drag
00079
00080     //DampFlag = 1. LAMMPS version
00081     if(DampFlag == 1){
00082     nodeDragx[atom1ID] =  fdVal * dr[1];  //node-node drag  //Important change made on 03Apr2025.
    Mention it in GitHub
00083     nodeDragy[atom1ID] =  fdVal * dr[2];  //node-node drag  //Adding the drag forces is wrong. Only add
    the
00084     nodeDragx[atom2ID] =  -fdVal * dr[1];  //node-node drag //total force
00085     nodeDragy[atom2ID] =  -fdVal * dr[2];  //node-node drag
00086
00087     ax[atom1ID] +=  (fcVal + fdVal) * dr[1];
00088     ay[atom1ID] +=  (fcVal + fdVal) * dr[2];
00089     ax[atom2ID] += -(fcVal + fdVal) * dr[1];
00090     ay[atom2ID] += -(fcVal + fdVal) * dr[2];
00091     }
00092
00093     //DampFlag = 2. Suzanne notes version
00094     else if(DampFlag == 2){
00095     nodeDragx[atom1ID] =  -gamman * vr[1];  //node-node drag
00096     nodeDragy[atom1ID] =  -gamman * vr[2]; //node-node drag
00097     nodeDragx[atom2ID] =  -(-gamman * vr[1]);  //node-node drag
00098     nodeDragy[atom2ID] =  -(-gamman * vr[2]);  //node-node drag
00099
00100     ax[atom1ID] +=  (fcVal * dr[1] - gamman * vr[1]);
00101     ay[atom1ID] +=  (fcVal * dr[2] - gamman * vr[2]);
00102     ax[atom2ID] += -(fcVal * dr[1] - gamman * vr[1]);
00103     ay[atom2ID] += -(fcVal * dr[2] - gamman * vr[2]);
00104     }
00105
00106     //DampFlag = 3. Suzanne PRL, 130, 178203 (2023) version
00107     else if(DampFlag == 3){
00108      DeltaXijNew = dr[1];
00109      DeltaYijNew = dr[2];
00110
00111      if(stepCount == 0) {  // First timestep
00112       DeltaXijOld[n] = DeltaXijNew;
00113       DeltaYijOld[n] = DeltaYijNew;
00114      }
00115
00116      DeltaXij = DeltaXijNew - DeltaXijOld[n];
00117      DeltaYij = DeltaYijNew - DeltaYijOld[n];
00118      DeltaVXij = DeltaXij / deltaT;
00119      DeltaVYij = DeltaYij / deltaT;
00120
00121      // Now update for the next timestep
00122      DeltaXijOld[n] = DeltaXijNew;
00123      DeltaYijOld[n] = DeltaYijNew;
00124
00125      nodeDragx[atom1ID] =  -gamman * DeltaVXij;  //node-node drag
00126      nodeDragy[atom1ID] =  -gamman * DeltaVYij; //node-node drag
00127      nodeDragx[atom2ID] =  -(-gamman * DeltaVXij);  //node-node drag
00128      nodeDragy[atom2ID] =  -(-gamman * DeltaVYij);  //node-node drag
00129
00130      ax[atom1ID] +=  (fcVal * dr[1] - gamman * DeltaVXij);
00131      ay[atom1ID] +=  (fcVal * dr[2] - gamman * DeltaVYij);
00132      ax[atom2ID] += -(fcVal * dr[1] - gamman * DeltaVXij);
00133      ay[atom2ID] += -(fcVal * dr[2] - gamman * DeltaVYij);
00134     }
00135
00136
00137     BondLength[n] = r;
00138     BondEnergy[n] = uVal; //No 0.5 factor since it is the energy of the bond
00139     TotalBondEnergy   +=  BondEnergy[n];
00140
00141     virSumBond +=   0.5 * (fcVal + fdVal) * rr;
00142     virSumBondxx += 0.5 * (fcVal + fdVal) * dr[1] * dr[1];
```

```
00143     virSumBondyy += 0.5 * (fcVal + fdVal) * dr[2] * dr[2];
00144     virSumBondxy += 0.5 * (fcVal + fdVal) * dr[1] * dr[2];
00145 } }
```

3.26 source/ComputeBondForce.h File Reference

This graph shows which files directly or indirectly include this file:



Functions

- void ComputeBondForce ()

3.26.1 Function Documentation

3.26.1.1 ComputeBondForce()

```
void ComputeBondForce ( )
```

Definition at line 28 of file ComputeBondForce.c.

```
00028                           {
00029   int n;
00030   double dr[NDIM+1], r, rr, ri, roi;
00031   double uVal, fcVal;
00032
00033   uVal = 0.0; TotalBondEnergy = 0.0;
00034   virSumBond = 0.0; virSumBondxx = 0.0; virSumBondyy = 0.0; virSumBondxy = 0.0;
00035
00036   double vr[NDIM+1], fdVal, rri;
00037
00038   for(n = 1 ; n <= nAtom ; n ++){
00039    nodeDragx[n] = 0.0;
00040    nodeDragy[n] = 0.0;
00041   } //Important change made on 03Apr2025. Mention it in GitHub
00042
00043   int atom1ID, atom2ID;
00044
00045   for(n=1; n<=nBond; n++){
00046    rr = 0.0; rri = 0.0; fcVal = 0.0;  fdVal = 0.0; strech = 0.0;
00047    atom1ID = atom1[n];
00048    atom2ID = atom2[n];
00049
00050    dr[1] = rx[atom1ID] - rx[atom2ID];
00051    if(dr[1] >= regionH[1])
00052     dr[1] -= region[1];
00053    else if(dr[1] < -regionH[1])
00054     dr[1] += region[1];
00055
```

```
00056     dr[2] = ry[atom1ID] - ry[atom2ID];
00057     if(dr[2] >= regionH[2]){
00058      dr[1] -= shearDisplacement;
00059      if(dr[1] < -regionH[1]) dr[1] += region[1];
00060      dr[2] -= region[2];
00061    }else if(dr[2] < -regionH[2]){
00062     dr[1] += shearDisplacement;
00063      if(dr[1] >= regionH[1]) dr[1] -= region[1];
00064     dr[2] += region[2];
00065    }
00066
00067     rr = Sqr(dr[1]) + Sqr(dr[2]);
00068     r = sqrt(rr);
00069     rri = 1.0/rr;
00070     ri = 1.0/r;
00071     roi = 1.0/ro[n];
00072     strech = (r * roi - 1.0);
00073     uVal = 0.5 * kb[n] * ro[n] * Sqr(strech);
00074     fcVal = -kb[n] * strech * ri; //F = -Grad U
00075
00076     vr[1] = vx[atom1ID] - vx[atom2ID];
00077     vr[2] = vy[atom1ID] - vy[atom2ID];
00078     fdVal = -gamman * (vr[1]*dr[1] + vr[2]*dr[2]) * rri; //node-node drag
00079
00080     //DampFlag = 1. LAMMPS version
00081     if(DampFlag == 1){
00082     nodeDragx[atom1ID] =  fdVal * dr[1];  //node-node drag  //Important change made on 03Apr2025.
    Mention it in GitHub
00083     nodeDragy[atom1ID] =  fdVal * dr[2];  //node-node drag  //Adding the drag forces is wrong. Only add
    the
00084     nodeDragx[atom2ID] =  -fdVal * dr[1];  //node-node drag //total force
00085     nodeDragy[atom2ID] =  -fdVal * dr[2];  //node-node drag
00086
00087     ax[atom1ID] +=  (fcVal + fdVal) * dr[1];
00088     ay[atom1ID] +=  (fcVal + fdVal) * dr[2];
00089     ax[atom2ID] += -(fcVal + fdVal) * dr[1];
00090     ay[atom2ID] += -(fcVal + fdVal) * dr[2];
00091     }
00092
00093     //DampFlag = 2. Suzanne notes version
00094     else if(DampFlag == 2){
00095     nodeDragx[atom1ID] =  -gamman * vr[1];  //node-node drag
00096     nodeDragy[atom1ID] =  -gamman * vr[2]; //node-node drag
00097     nodeDragx[atom2ID] =  -(-gamman * vr[1]);  //node-node drag
00098     nodeDragy[atom2ID] =  -(-gamman * vr[2]);  //node-node drag
00099
00100     ax[atom1ID] +=  (fcVal * dr[1] - gamman * vr[1]);
00101     ay[atom1ID] +=  (fcVal * dr[2] - gamman * vr[2]);
00102     ax[atom2ID] += -(fcVal * dr[1] - gamman * vr[1]);
00103     ay[atom2ID] += -(fcVal * dr[2] - gamman * vr[2]);
00104     }
00105
00106     //DampFlag = 3. Suzanne PRL, 130, 178203 (2023) version
00107     else if(DampFlag == 3){
00108      DeltaXijNew = dr[1];
00109      DeltaYijNew = dr[2];
00110
00111      if(stepCount == 0) {  // First timestep
00112       DeltaXijOld[n] = DeltaXijNew;
00113       DeltaYijOld[n] = DeltaYijNew;
00114      }
00115
00116      DeltaXij = DeltaXijNew - DeltaXijOld[n];
00117      DeltaYij = DeltaYijNew - DeltaYijOld[n];
00118      DeltaVXij = DeltaXij / deltaT;
00119      DeltaVYij = DeltaYij / deltaT;
00120
00121      // Now update for the next timestep
00122      DeltaXijOld[n] = DeltaXijNew;
00123      DeltaYijOld[n] = DeltaYijNew;
00124
00125      nodeDragx[atom1ID] =  -gamman * DeltaVXij;  //node-node drag
00126      nodeDragy[atom1ID] =  -gamman * DeltaVYij; //node-node drag
00127      nodeDragx[atom2ID] =  -(-gamman * DeltaVXij);  //node-node drag
00128      nodeDragy[atom2ID] =  -(-gamman * DeltaVYij);  //node-node drag
00129
00130      ax[atom1ID] +=  (fcVal * dr[1] - gamman * DeltaVXij);
00131      ay[atom1ID] +=  (fcVal * dr[2] - gamman * DeltaVYij);
00132      ax[atom2ID] += -(fcVal * dr[1] - gamman * DeltaVXij);
00133      ay[atom2ID] += -(fcVal * dr[2] - gamman * DeltaVYij);
00134     }
00135
00136
00137     BondLength[n] = r;
00138     BondEnergy[n] = uVal; //No 0.5 factor since it is the energy of the bond
00139     TotalBondEnergy   +=  BondEnergy[n];
00140
```

```
00141     virSumBond +=   0.5 * (fcVal + fdVal) * rr;
00142     virSumBondxx += 0.5 * (fcVal + fdVal) * dr[1] * dr[1];
00143     virSumBondyy += 0.5 * (fcVal + fdVal) * dr[2] * dr[2];
00144     virSumBondxy += 0.5 * (fcVal + fdVal) * dr[1] * dr[2];
00145 } }
```

References atom1, atom2, ax, ay, BondEnergy, BondLength, DampFlag, deltaT, DeltaVXij, DeltaVYij, DeltaXij, DeltaXijNew, DeltaXijOld, DeltaYij, DeltaYijNew, DeltaYijOld, gamman, kb, nAtom, nBond, NDIM, nodeDragx, nodeDragy, region, regionH, ro, rx, ry, shearDisplacement, Sqr, stepCount, strech, TotalBondEnergy, virSumBond, virSumBondxx, virSumBondxy, virSumBondyy, vx, and vy.

Referenced by main().

Here is the caller graph for this function:

3.27 ComputeBondForce.h

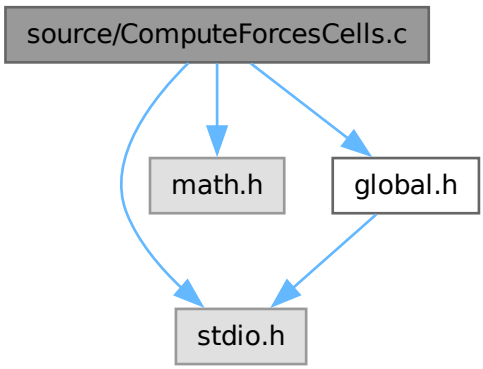
Go to the documentation of this file.

```
00001 #ifndef COMPUTE_BOND_FORCE_H
00002 #define COMPUTE_BOND_FORCE_H
00003
00004 void ComputeBondForce();
00005
00006 #endif
00007
```

3.28 source/ComputeForcesCells.c File Reference

```
#include <stdio.h>
#include <math.h>
#include "global.h"
```

Include dependency graph for ComputeForcesCells.c:



Functions

- void ComputeForcesCells ()

3.28.1 Function Documentation

3.28.1.1 ComputeForcesCells()

```
void ComputeForcesCells ( )
```

Definition at line 25 of file ComputeForcesCells.c.

```
00025                           {
00026   double dr[NDIM+1], invWid[NDIM+1], shift[NDIM+1], f, fcVal, rr, ri, r, uVal;
00027   int c, I, J, m1, m1X, m1Y, m2, m2X, m2Y, n, offset;
00028   int iofX[] = {0, 0, 1, 1, 0, -1, -1, -1, 0, 1},
00029       iofY[] = {0, 0, 0, 1 ,1, 1, 0, -1, -1, -1};
00030
00031   invWid[1] = cells[1]/region[1];
00032   invWid[2] = cells[2]/region[2];
00033
00034   for(n = nAtom+1; n <= nAtom+cells[1]*cells[2] ; n++)
00035     cellList[n] = 0;
00036
00037   for(n = 1 ; n <= nAtom ; n ++){
00038     c = ((int)((ry[n] + regionH[2])*invWid[2]))*cells[1] + (int)((rx[n]+regionH[1])*invWid[1]) +
      nAtom+ 1;
00039     cellList[n] = cellList[c];
00040     cellList[c] = n;
00041   }
00042
00043   for(n = 1 ; n <= nAtom ; n ++){
00044     ax[n] = 0.;
00045     ay[n] = 0.;
00046   }
00047
00048   uSum = 0.0 ;
00049   virSum = 0.0;
00050   rfAtom = 0.0;
00051   RadiusIJ = 0.0;
00052
00053   gamman = 1.0;
00054   double vr[NDIM+1], fd, fdVal, rrinv;
00055   rrinv = 0.0;
00056   fd = 0.0;
```

```
00057   fdVal = 0.0;
00058
00059   int start = 1 + rank*(cells[2]/size);
00060   int end = (rank+1)*(cells[2]/size);
00061
00062   for(m1Y = start ; m1Y <= end ; m1Y ++){
00063     for(m1X = 1 ; m1X <= cells[1] ; m1X ++){
00064       m1 = (m1Y-1) * cells[1] + m1X + nAtom;
00065       for(offset = 1 ; offset <= 9 ; offset ++){
00066     m2X = m1X + iofX[offset]; shift[1] = 0.;
00067     if(m2X > cells[1]){
00068       m2X = 1; shift[1] = region[1];
00069     }else if(m2X == 0){
00070       m2X = cells[1]; shift[1] = -region[1];
00071     }
00072     m2Y = m1Y + iofY[offset]; shift[2] = 0.;
00073     if(m2Y > cells[2]){
00074       m2Y = 1; shift[2] = region[2];
00075     }else if(m2Y == 0){
00076       m2Y = cells[2]; shift[2] = -region[2];
00077     }
00078     m2 = (m2Y-1)*cells[1] + m2X + nAtom;
00079     I = cellList[m1];
00080     while(I > 0){
00081       J = cellList[m2];
00082       while(J > 0){
00083         if(m1 == m2 && J != I && (atomRadius[I] > 0. && atomRadius[J] > 0.)){
00084           dr[1] = rx[I] - rx[J] - shift[1];
00085           dr[2] = ry[I] - ry[J] - shift[2];
00086           rr = Sqr(dr[1]) + Sqr(dr[2]);
00087           RadiusIJ = atomRadius[I] + atomRadius[J];
00088           SqrRadiusIJ = Sqr(RadiusIJ);
00089           if(rr < SqrRadiusIJ){
00090         r = sqrt(rr);
00091         ri = 1.0/r;
00092                 rrinv = 1.0/rr;
00093                 vr[1] = vx[I] - vx[J];
00094                 vr[2] = vy[I] - vy[J];
00095         RadiusIJInv = 1.0/RadiusIJ;
00096         uVal = Sqr(1.0 - r * RadiusIJInv);
00097         fcVal = 2.0 * RadiusIJInv * (1.0 - r * RadiusIJInv) *ri;
00098                 fdVal = -gamman * (vr[1]*dr[1] + vr[2]*dr[2]) * rrinv; //disc-disc drag
00099
00100         f  = fcVal * dr[1];
00101                 fd = fdVal * dr[1];
00102         ax[I] += (f + fd);
00103                 discDragx[I] += fd; //disc-disc drag
00104
00105         f = fcVal * dr[2];
00106                 fd = fdVal * dr[2];
00107         ay[I] += (f + fd);
00108                 discDragy[I] += fd; //disc-disc drag
00109
00110         uSum +=  0.5 * uVal;
00111         virSum += 0.5 * fcVal * rr;
00112         rfAtom += 0.5 * dr[1] * fcVal * dr[2];
00113           }
00114         }else if(m1 != m2 && (atomRadius[I] > 0. && atomRadius[J] > 0.)){
00115           dr[1] = rx[I] - rx[J] - shift[1];
00116           dr[2] = ry[I] - ry[J] - shift[2];
00117           rr = Sqr(dr[1]) + Sqr(dr[2]);
00118           RadiusIJ = atomRadius[I] + atomRadius[J];
00119           SqrRadiusIJ = Sqr(RadiusIJ);
00120           if(rr < SqrRadiusIJ){
00121         r = sqrt(rr);
00122         ri = 1.0/r;
00123                 rrinv = 1.0/r;
00124                 vr[1] = vx[I] - vx[J];
00125                 vr[2] = vy[I] - vy[J];
00126         RadiusIJInv = 1.0/RadiusIJ;
00127         uVal = Sqr(1.0 - r * RadiusIJInv);
00128         fcVal = 2.0 * RadiusIJInv * (1.0 - r * RadiusIJInv) *ri;
00129                 fdVal = -gamman * (vr[1]*dr[1] + vr[2]*dr[2]) * rrinv; //disc-disc drag
00130
00131         f  = fcVal * dr[1];
00132                 fd =  fdVal * dr[1];
00133         ax[I] += (f + fd);
00134                 discDragx[I] += fd; //disc-disc drag
00135
00136         f  = fcVal * dr[2];
00137                 fd = fdVal * dr[2];
00138         ay[I] += (f + fd);
00139                 discDragy[I] += fd; //disc-disc drag
00140
00141         uSum +=  0.5 * uVal;
00142         virSum += 0.5 * fcVal * rr;
00143         rfAtom += 0.5 * dr[1] * fcVal * dr[2];
```

```
00144           }
00145         }
00146             J = cellList[J];
00147       }
00148       I = cellList[I];
00149     }
00150       }
00151     }
00152   }
00153 }
```

References atomRadius, ax, ay, cellList, cells, discDragx, discDragy, gamman, nAtom, NDIM, RadiusIJ, RadiusIJInv, rank, region, regionH, rfAtom, rx, ry, size, Sqr, SqrRadiusIJ, uSum, virSum, vx, and vy.

3.29 ComputeForcesCells.c

Go to the documentation of this file.

```
00001 /*
00002  * This file is part of Lamina.
00003  *
00004  * Lamina is free software: you can redistribute it and/or modify
00005  * it under the terms of the GNU General Public License as published by
00006  * the Free Software Foundation, either version 3 of the License, or
00007  * (at your option) any later version.
00008  *
00009  * Lamina is distributed in the hope that it will be useful,
00010  * but WITHOUT ANY WARRANTY; without even the implied warranty of
00011  * MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the
00012  * GNU General Public License for more details.
00013  *
00014  * You should have received a copy of the GNU General Public License
00015  * along with Lamina. If not, see <https://www.gnu.org/licenses/>.
00016
00017  Copyright (C) 2025 Harish Charan, University of Durham, UK
00018
00019  */
00020
00021 #include<stdio.h>
00022 #include<math.h>
00023 #include"global.h"
00024
00025 void ComputeForcesCells(){
00026   double dr[NDIM+1], invWid[NDIM+1], shift[NDIM+1], f, fcVal, rr, ri, r, uVal;
00027   int c, I, J, m1, m1X, m1Y, m2, m2X, m2Y, n, offset;
00028   int iofX[] = {0, 0, 1, 1, 0, -1, -1, -1, 0, 1},
00029       iofY[] = {0, 0, 0, 1 ,1, 1, 0, -1, -1, -1};
00030
00031   invWid[1] = cells[1]/region[1];
00032   invWid[2] = cells[2]/region[2];
00033
00034   for(n = nAtom+1; n <= nAtom+cells[1]*cells[2] ; n++)
00035     cellList[n] = 0;
00036
00037   for(n = 1 ; n <= nAtom ; n ++){
00038     c = ((int)((ry[n] + regionH[2])*invWid[2]))*cells[1] + (int)((rx[n]+regionH[1])*invWid[1]) +
    nAtom+ 1;
00039     cellList[n] = cellList[c];
00040     cellList[c] = n;
00041   }
00042
00043   for(n = 1 ; n <= nAtom ; n ++){
00044     ax[n] = 0.;
00045     ay[n] = 0.;
00046   }
00047
00048   uSum = 0.0 ;
00049   virSum = 0.0;
00050   rfAtom = 0.0;
00051   RadiusIJ = 0.0;
00052
00053   gamman = 1.0;
00054   double vr[NDIM+1], fd, fdVal, rrinv;
00055   rrinv = 0.0;
00056   fd = 0.0;
00057   fdVal = 0.0;
00058
00059   int start = 1 + rank*(cells[2]/size);
00060   int end = (rank+1)*(cells[2]/size);
00061
00062   for(m1Y = start ; m1Y <= end ; m1Y ++){
```

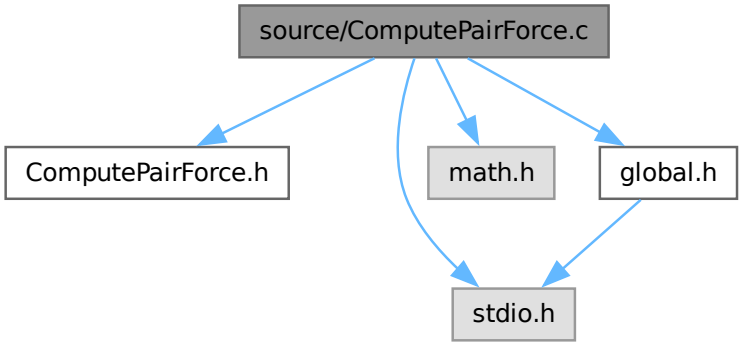
```
00063     for(m1X = 1 ; m1X <= cells[1] ; m1X ++){
00064       m1 = (m1Y-1) * cells[1] + m1X + nAtom;
00065       for(offset = 1 ; offset <= 9 ; offset ++){
00066     m2X = m1X + iofX[offset]; shift[1] = 0.;
00067     if(m2X > cells[1]){
00068       m2X = 1; shift[1] = region[1];
00069     }else if(m2X == 0){
00070       m2X = cells[1]; shift[1] = -region[1];
00071     }
00072     m2Y = m1Y + iofY[offset]; shift[2] = 0.;
00073     if(m2Y > cells[2]){
00074       m2Y = 1; shift[2] = region[2];
00075     }else if(m2Y == 0){
00076       m2Y = cells[2]; shift[2] = -region[2];
00077     }
00078     m2 = (m2Y-1)*cells[1] + m2X + nAtom;
00079     I = cellList[m1];
00080     while(I > 0){
00081       J = cellList[m2];
00082       while(J > 0){
00083         if(m1 == m2 && J != I && (atomRadius[I] > 0. && atomRadius[J] > 0.)){
00084           dr[1] = rx[I] - rx[J] - shift[1];
00085           dr[2] = ry[I] - ry[J] - shift[2];
00086           rr = Sqr(dr[1]) + Sqr(dr[2]);
00087           RadiusIJ = atomRadius[I] + atomRadius[J];
00088           SqrRadiusIJ = Sqr(RadiusIJ);
00089           if(rr < SqrRadiusIJ){
00090         r = sqrt(rr);
00091         ri = 1.0/r;
00092                 rrinv = 1.0/rr;
00093                 vr[1] = vx[I] - vx[J];
00094                 vr[2] = vy[I] - vy[J];
00095         RadiusIJInv = 1.0/RadiusIJ;
00096         uVal = Sqr(1.0 - r * RadiusIJInv);
00097         fcVal = 2.0 * RadiusIJInv * (1.0 - r * RadiusIJInv) *ri;
00098                 fdVal = -gamman * (vr[1]*dr[1] + vr[2]*dr[2]) * rrinv; //disc-disc drag
00099
00100         f  = fcVal * dr[1];
00101                 fd = fdVal * dr[1];
00102         ax[I] += (f + fd);
00103                 discDragx[I] += fd; //disc-disc drag
00104
00105         f = fcVal * dr[2];
00106                 fd = fdVal * dr[2];
00107         ay[I] += (f + fd);
00108                 discDragy[I] += fd; //disc-disc drag
00109
00110         uSum +=  0.5 * uVal;
00111         virSum += 0.5 * fcVal * rr;
00112         rfAtom += 0.5 * dr[1] * fcVal * dr[2];
00113           }
00114         }else if(m1 != m2 && (atomRadius[I] > 0. && atomRadius[J] > 0.)){
00115           dr[1] = rx[I] - rx[J] - shift[1];
00116           dr[2] = ry[I] - ry[J] - shift[2];
00117           rr = Sqr(dr[1]) + Sqr(dr[2]);
00118           RadiusIJ = atomRadius[I] + atomRadius[J];
00119           SqrRadiusIJ = Sqr(RadiusIJ);
00120           if(rr < SqrRadiusIJ){
00121         r = sqrt(rr);
00122         ri = 1.0/r;
00123                 rrinv = 1.0/r;
00124                 vr[1] = vx[I] - vx[J];
00125                 vr[2] = vy[I] - vy[J];
00126         RadiusIJInv = 1.0/RadiusIJ;
00127         uVal = Sqr(1.0 - r * RadiusIJInv);
00128         fcVal = 2.0 * RadiusIJInv * (1.0 - r * RadiusIJInv) *ri;
00129                 fdVal = -gamman * (vr[1]*dr[1] + vr[2]*dr[2]) * rrinv; //disc-disc drag
00130
00131         f  = fcVal * dr[1];
00132                 fd =  fdVal * dr[1];
00133         ax[I] += (f + fd);
00134                 discDragx[I] += fd; //disc-disc drag
00135
00136         f  = fcVal * dr[2];
00137                 fd = fdVal * dr[2];
00138         ay[I] += (f + fd);
00139                 discDragy[I] += fd; //disc-disc drag
00140
00141         uSum +=  0.5 * uVal;
00142         virSum += 0.5 * fcVal * rr;
00143         rfAtom += 0.5 * dr[1] * fcVal * dr[2];
00144           }
00145         }
00146             J = cellList[J];
00147       }
00148       I = cellList[I];
00149     }
```

```
00150       }
00151     }
00152   }
00153 }
```

3.30 source/ComputePairForce.c File Reference

```
#include "ComputePairForce.h"
#include <stdio.h>
#include <math.h>
#include "global.h"
```

Include dependency graph for ComputePairForce.c:



Functions

- void ComputePairForce (int normFlag)

3.30.1 Function Documentation

3.30.1.1 ComputePairForce()

```
void ComputePairForce (
            int normFlag )
```

Definition at line 27 of file ComputePairForce.c.

```
00027                                   {
00028 double dr[NDIM+1], fcVal, rr, ri, r, uVal;
00029 int n, i,j;
00030 uVal = 0.0;  uSumPair = 0.0 ;
00031 virSumPair = 0.0; virSumPairxx = 0.0; virSumPairyy = 0.0; virSumPairxy = 0.0;
00032
00033 for(n = 1 ; n <= nAtom ; n ++){
00034  ax[n] = 0.0;
00035  ay[n] = 0.0;
00036  discDragx[n] = 0.0;
00037  discDragy[n] = 0.0;
00038 }
00039 for(n = 1; n <= nPairTotal; n ++){
00040  PairID[n] = 0;
```

```
00041  Pairatom1[n] = 0;
00042  Pairatom2[n] = 0;
00043  PairXij[n] = 0.0;
00044  PairYij[n] = 0.0;
00045 }
00046
00047
00048 Kn = 1.0;
00049 double vr[NDIM+1], fdVal, rri;
00050 nPairActive = 0;
00051 double meff;
00052 meff = 0.0;
00053 int atomIDi, atomIDj;
00054 //int processThisPair = 1;
00055
00056 for(i=1;i<=nAtomInterface;i++){
00057  for(j=i+1;j<=nAtomInterface;j++){
00058   atomIDi = atomIDInterface[i];
00059   atomIDj = atomIDInterface[j];
00060   if (isBonded[atomIDi][atomIDj] == 0) { //To exclude pair interaction between bonded atoms
00061   rr = 0.0; rri = 0.0; fcVal = 0.0;  fdVal = 0.0; strech = 0.0;
00062   RadiusIJ = 0.0;
00063
00064   dr[1] = rx[atomIDi] - rx[atomIDj];
00065   if(dr[1] >= regionH[1])
00066    dr[1] -= region[1];
00067   else if(dr[1] < -regionH[1])
00068     dr[1] += region[1];
00069
00070   dr[2] = ry[atomIDi] - ry[atomIDj];
00071    if(dr[2] >= regionH[2]){
00072     dr[1] -= shearDisplacement;
00073     if(dr[1] < -regionH[1]) dr[1] += region[1];
00074     dr[2] -= region[2];
00075   }else if(dr[2] < -regionH[2]){
00076    dr[1] += shearDisplacement;
00077     if(dr[1] >= regionH[1]) dr[1] -= region[1];
00078    dr[2] += region[2];
00079   }
00080
00081   rr = Sqr(dr[1]) + Sqr(dr[2]);
00082   RadiusIJ = atomRadius[atomIDi] + atomRadius[atomIDj];
00083   SqrRadiusIJ = Sqr(RadiusIJ);
00084   if(rr < SqrRadiusIJ){
00085    r = sqrt(rr);
00086    ri = 1.0/r;
00087    rri = 1.0/rr;
00088    RadiusIJInv = 1.0/RadiusIJ;
00089    strech = (RadiusIJ - r);
00090    uVal = 0.5 * Kn * Sqr(strech);
00091
00092    //NormFlag
00093    if(normFlag == 1){
00094     strech = strech * RadiusIJInv;
00095     uVal = 0.5 * Kn * RadiusIJ * Sqr(strech);
00096     }
00097
00098    fcVal = Kn * strech * ri;
00099    vr[1] = vx[atomIDi] - vx[atomIDj];
00100   vr[2] = vy[atomIDi] - vy[atomIDj];
00101
00102   nPairActive++;
00103   PairID[nPairActive] = nPairActive;
00104   Pairatom1[nPairActive] = atomIDi;
00105   Pairatom2[nPairActive] = atomIDj;
00106   PairXij[nPairActive] = dr[1];
00107   PairYij[nPairActive] = dr[2];
00108
00109   //DampFlag = 1
00110   if(DampFlag == 1){
00111   meff = (atomMass[atomIDi]*atomMass[atomIDj])/(atomMass[atomIDi] + atomMass[atomIDj]);
00112   fdVal = -gamman * meff * (vr[1]*dr[1] + vr[2]*dr[2]) * rri; //disc-disc drag
00113
00114   discDragx[atomIDi] =  fdVal * dr[1]; //disc-disc drag
00115   discDragy[atomIDi] =  fdVal * dr[2]; //disc-disc drag
00116   discDragx[atomIDj] = -fdVal * dr[1]; //disc-disc drag
00117   discDragy[atomIDj] = -fdVal * dr[2]; //disc-disc drag
00118
00119   discDragx[nPairActive] = discDragx[atomIDi];
00120   discDragy[nPairActive] = discDragy[atomIDi];
00121
00122
00123   ax[atomIDi] += (fcVal + fdVal) * dr[1];
00124   ay[atomIDi] += (fcVal + fdVal) * dr[2];
00125   ax[atomIDj] += -(fcVal + fdVal) * dr[1];
00126   ay[atomIDj] += -(fcVal + fdVal) * dr[2];
00127  }
```

```
00128
00129   //DampFlag = 2
00130   else if(DampFlag == 2){
00131    discDragx[atomIDi] =  -gamman * vr[1]; //disc-disc drag
00132    discDragy[atomIDi] =  -gamman * vr[2]; //disc-disc drag
00133    discDragx[atomIDj] = -(-gamman * vr[1]); //disc-disc drag
00134    discDragy[atomIDj] = -(-gamman * vr[2]); //disc-disc drag
00135
00136    discDragx[nPairActive] = discDragx[atomIDi];
00137    discDragy[nPairActive] = discDragy[atomIDi];
00138
00139
00140    ax[atomIDi] +=  (fcVal * dr[1] - gamman * vr[1]);
00141    ay[atomIDi] +=  (fcVal * dr[2] - gamman * vr[2]);
00142    ax[atomIDj] += -(fcVal * dr[1] - gamman * vr[1]);
00143    ay[atomIDj] += -(fcVal * dr[2] - gamman * vr[2]);
00144   }
00145
00146   //DampFlag = 3. Suzanne PRL, 130, 178203 (2023) version
00147   else if(DampFlag == 3){
00148   //Track compression velocity
00149   DeltaXijNew = dr[1];
00150   DeltaYijNew = dr[2];
00151   if(stepCount == 0) { // Initialization step
00152    DeltaXijOldPair[atomIDi][atomIDj] = DeltaXijNew;
00153    DeltaYijOldPair[atomIDi][atomIDj] = DeltaYijNew;
00154    }
00155
00156    DeltaXij = DeltaXijNew - DeltaXijOldPair[atomIDi][atomIDj];
00157    DeltaYij = DeltaYijNew - DeltaYijOldPair[atomIDi][atomIDj];
00158    DeltaVXij = DeltaXij / deltaT;
00159    DeltaVYij = DeltaYij / deltaT;
00160
00161    // Update history for next step
00162    DeltaXijOldPair[atomIDi][atomIDj] = DeltaXijNew;
00163    DeltaYijOldPair[atomIDi][atomIDj] = DeltaYijNew;
00164
00165    discDragx[atomIDi] =  -gamman * DeltaVXij; //disc-disc drag
00166    discDragy[atomIDi] =  -gamman * DeltaVYij; //disc-disc drag
00167    discDragx[atomIDj] = -(-gamman * DeltaVXij); //disc-disc drag
00168    discDragy[atomIDj] = -(-gamman * DeltaVYij); //disc-disc drag
00169
00170    discDragx[nPairActive] = discDragx[atomIDi];
00171    discDragy[nPairActive] = discDragy[atomIDi];
00172
00173    ax[atomIDi] +=  (fcVal * dr[1] - gamman * DeltaVXij);
00174    ay[atomIDi] +=  (fcVal * dr[2] - gamman * DeltaVYij);
00175    ax[atomIDj] += -(fcVal * dr[1] - gamman * DeltaVXij);
00176    ay[atomIDj] += -(fcVal * dr[2] - gamman * DeltaVYij);
00177   }
00178
00179   //In the following, for stress/virial term (fcVal + fdVal) is used since the total pair force =
      Hookean Interaction + relative velocity drag
00180   uSumPair +=  0.5 * uVal;
00181   virSumPair += 0.5 * (fcVal + fdVal) * rr;
00182   virSumPairxx += 0.5 * (fcVal + fdVal) * dr[1] * dr[1];
00183   virSumPairyy += 0.5 * (fcVal + fdVal) * dr[2] * dr[2];
00184   virSumPairxy += 0.5 * (fcVal + fdVal) * dr[1] * dr[2];
00185     }
00186   else { //Resetting the distance between two discs when they are not in contact
00187    DeltaXijOldPair[atomIDi][atomIDj] = 0.0;
00188    DeltaYijOldPair[atomIDi][atomIDj] = 0.0;
00189    DeltaXijOldPair[atomIDj][atomIDi] = 0.0;
00190    DeltaYijOldPair[atomIDj][atomIDi] = 0.0;
00191     }
00192    }
00193   }
00194  }
00195 }
```

References atomIDInterface, atomMass, atomRadius, ax, ay, DampFlag, deltaT, DeltaVXij, DeltaVYij, DeltaXij, DeltaXijNew, DeltaXijOldPair, DeltaYij, DeltaYijNew, DeltaYijOldPair, discDragx, discDragy, gamman, isBonded, Kn, nAtom, nAtomInterface, NDIM, nPairActive, nPairTotal, Pairatom1, Pairatom2, PairID, PairXij, PairYij, RadiusIJ, RadiusIJInv, region, regionH, rx, ry, shearDisplacement, Sqr, SqrRadiusIJ, stepCount, strech, uSumPair, virSumPair, virSumPairxx, virSumPairxy, virSumPairyy, vx, and vy.

Referenced by main().

Here is the caller graph for this function:

3.31 ComputePairForce.c

Go to the documentation of this file.

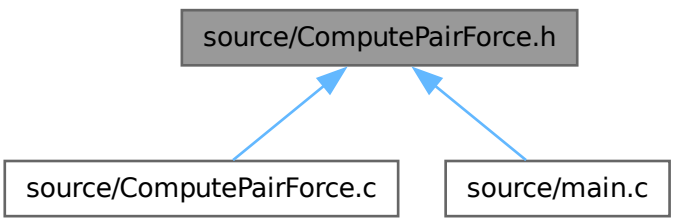
```
00001 /*
00002  * This file is part of Lamina.
00003  *
00004  * Lamina is free software: you can redistribute it and/or modify
00005  * it under the terms of the GNU General Public License as published by
00006  * the Free Software Foundation, either version 3 of the License, or
00007  * (at your option) any later version.
00008  *
00009  * Lamina is distributed in the hope that it will be useful,
00010  * but WITHOUT ANY WARRANTY; without even the implied warranty of
00011  * MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the
00012  * GNU General Public License for more details.
00013  *
00014  * You should have received a copy of the GNU General Public License
00015  * along with Lamina. If not, see <https://www.gnu.org/licenses/>.
00016
00017  Copyright (C) 2025 Harish Charan, University of Durham, UK
00018
00019  */
00020
00021 #include "ComputePairForce.h"
00022
00023 #include<stdio.h>
00024 #include<math.h>
00025 #include"global.h"
00026
00027 void ComputePairForce(int normFlag){
00028 double dr[NDIM+1], fcVal, rr, ri, r, uVal;
00029 int n, i,j;
00030 uVal = 0.0;  uSumPair = 0.0 ;
00031 virSumPair = 0.0; virSumPairxx = 0.0; virSumPairyy = 0.0; virSumPairxy = 0.0;
00032
00033 for(n = 1 ; n <= nAtom ; n ++){
00034  ax[n] = 0.0;
00035  ay[n] = 0.0;
00036  discDragx[n] = 0.0;
00037  discDragy[n] = 0.0;
00038 }
00039 for(n = 1; n <= nPairTotal; n ++){
00040  PairID[n] = 0;
00041  Pairatom1[n] = 0;
00042  Pairatom2[n] = 0;
00043  PairXij[n] = 0.0;
00044  PairYij[n] = 0.0;
00045 }
00046
00047
00048 Kn = 1.0;
00049 double vr[NDIM+1], fdVal, rri;
00050 nPairActive = 0;
00051 double meff;
00052 meff = 0.0;
00053 int atomIDi, atomIDj;
00054 //int processThisPair = 1;
00055
00056 for(i=1;i<=nAtomInterface;i++){
00057  for(j=i+1;j<=nAtomInterface;j++){
00058   atomIDi = atomIDInterface[i];
00059   atomIDj = atomIDInterface[j];
00060   if (isBonded[atomIDi][atomIDj] == 0) { //To exclude pair interaction between bonded atoms
```

```
00061   rr = 0.0; rri = 0.0; fcVal = 0.0;  fdVal = 0.0; strech = 0.0;
00062   RadiusIJ = 0.0;
00063
00064   dr[1] = rx[atomIDi] - rx[atomIDj];
00065   if(dr[1] >= regionH[1])
00066    dr[1] -= region[1];
00067   else if(dr[1] < -regionH[1])
00068     dr[1] += region[1];
00069
00070   dr[2] = ry[atomIDi] - ry[atomIDj];
00071    if(dr[2] >= regionH[2]){
00072     dr[1] -= shearDisplacement;
00073     if(dr[1] < -regionH[1]) dr[1] += region[1];
00074     dr[2] -= region[2];
00075   }else if(dr[2] < -regionH[2]){
00076    dr[1] += shearDisplacement;
00077     if(dr[1] >= regionH[1]) dr[1] -= region[1];
00078    dr[2] += region[2];
00079   }
00080
00081   rr = Sqr(dr[1]) + Sqr(dr[2]);
00082   RadiusIJ = atomRadius[atomIDi] + atomRadius[atomIDj];
00083   SqrRadiusIJ = Sqr(RadiusIJ);
00084   if(rr < SqrRadiusIJ){
00085    r = sqrt(rr);
00086    ri = 1.0/r;
00087    rri = 1.0/rr;
00088    RadiusIJInv = 1.0/RadiusIJ;
00089    strech = (RadiusIJ - r);
00090    uVal = 0.5 * Kn * Sqr(strech);
00091
00092    //NormFlag
00093    if(normFlag == 1){
00094     strech = strech * RadiusIJInv;
00095     uVal = 0.5 * Kn * RadiusIJ * Sqr(strech);
00096     }
00097
00098    fcVal = Kn * strech * ri;
00099    vr[1] = vx[atomIDi] - vx[atomIDj];
00100    vr[2] = vy[atomIDi] - vy[atomIDj];
00101
00102    nPairActive++;
00103    PairID[nPairActive] = nPairActive;
00104    Pairatom1[nPairActive] = atomIDi;
00105    Pairatom2[nPairActive] = atomIDj;
00106    PairXij[nPairActive] = dr[1];
00107    PairYij[nPairActive] = dr[2];
00108
00109    //DampFlag = 1
00110    if(DampFlag == 1){
00111    meff = (atomMass[atomIDi]*atomMass[atomIDj])/(atomMass[atomIDi] + atomMass[atomIDj]);
00112    fdVal = -gamman * meff * (vr[1]*dr[1] + vr[2]*dr[2]) * rri; //disc-disc drag
00113
00114    discDragx[atomIDi] =  fdVal * dr[1]; //disc-disc drag
00115    discDragy[atomIDi] =  fdVal * dr[2]; //disc-disc drag
00116    discDragx[atomIDj] = -fdVal * dr[1]; //disc-disc drag
00117    discDragy[atomIDj] = -fdVal * dr[2]; //disc-disc drag
00118
00119    discDragx[nPairActive] = discDragx[atomIDi];
00120    discDragy[nPairActive] = discDragy[atomIDi];
00121
00122
00123    ax[atomIDi] += (fcVal + fdVal) * dr[1];
00124    ay[atomIDi] += (fcVal + fdVal) * dr[2];
00125    ax[atomIDj] += -(fcVal + fdVal) * dr[1];
00126    ay[atomIDj] += -(fcVal + fdVal) * dr[2];
00127   }
00128
00129   //DampFlag = 2
00130   else if(DampFlag == 2){
00131    discDragx[atomIDi] =  -gamman * vr[1]; //disc-disc drag
00132    discDragy[atomIDi] =  -gamman * vr[2]; //disc-disc drag
00133    discDragx[atomIDj] = -(-gamman * vr[1]); //disc-disc drag
00134    discDragy[atomIDj] = -(-gamman * vr[2]); //disc-disc drag
00135
00136    discDragx[nPairActive] = discDragx[atomIDi];
00137    discDragy[nPairActive] = discDragy[atomIDi];
00138
00139
00140    ax[atomIDi] +=  (fcVal * dr[1] - gamman * vr[1]);
00141    ay[atomIDi] +=  (fcVal * dr[2] - gamman * vr[2]);
00142    ax[atomIDj] += -(fcVal * dr[1] - gamman * vr[1]);
00143    ay[atomIDj] += -(fcVal * dr[2] - gamman * vr[2]);
00144   }
00145
00146   //DampFlag = 3. Suzanne PRL, 130, 178203 (2023) version
00147   else if(DampFlag == 3){
```

```
00148   //Track compression velocity
00149   DeltaXijNew = dr[1];
00150   DeltaYijNew = dr[2];
00151   if(stepCount == 0) { // Initialization step
00152    DeltaXijOldPair[atomIDi][atomIDj] = DeltaXijNew;
00153    DeltaYijOldPair[atomIDi][atomIDj] = DeltaYijNew;
00154    }
00155
00156    DeltaXij = DeltaXijNew - DeltaXijOldPair[atomIDi][atomIDj];
00157    DeltaYij = DeltaYijNew - DeltaYijOldPair[atomIDi][atomIDj];
00158    DeltaVXij = DeltaXij / deltaT;
00159    DeltaVYij = DeltaYij / deltaT;
00160
00161    // Update history for next step
00162    DeltaXijOldPair[atomIDi][atomIDj] = DeltaXijNew;
00163    DeltaYijOldPair[atomIDi][atomIDj] = DeltaYijNew;
00164
00165    discDragx[atomIDi] =  -gamman * DeltaVXij; //disc-disc drag
00166    discDragy[atomIDi] =  -gamman * DeltaVYij; //disc-disc drag
00167    discDragx[atomIDj] = -(-gamman * DeltaVXij); //disc-disc drag
00168    discDragy[atomIDj] = -(-gamman * DeltaVYij); //disc-disc drag
00169
00170    discDragx[nPairActive] = discDragx[atomIDi];
00171    discDragy[nPairActive] = discDragy[atomIDi];
00172
00173    ax[atomIDi] +=  (fcVal * dr[1] - gamman * DeltaVXij);
00174    ay[atomIDi] +=  (fcVal * dr[2] - gamman * DeltaVYij);
00175    ax[atomIDj] += -(fcVal * dr[1] - gamman * DeltaVXij);
00176    ay[atomIDj] += -(fcVal * dr[2] - gamman * DeltaVYij);
00177   }
00178
00179   //In the following, for stress/virial term (fcVal + fdVal) is used since the total pair force =
      Hookean Interaction + relative velocity drag
00180   uSumPair +=  0.5 * uVal;
00181   virSumPair += 0.5 * (fcVal + fdVal) * rr;
00182   virSumPairxx += 0.5 * (fcVal + fdVal) * dr[1] * dr[1];
00183   virSumPairyy += 0.5 * (fcVal + fdVal) * dr[2] * dr[2];
00184   virSumPairxy += 0.5 * (fcVal + fdVal) * dr[1] * dr[2];
00185     }
00186   else { //Resetting the distance between two discs when they are not in contact
00187    DeltaXijOldPair[atomIDi][atomIDj] = 0.0;
00188    DeltaYijOldPair[atomIDi][atomIDj] = 0.0;
00189    DeltaXijOldPair[atomIDj][atomIDi] = 0.0;
00190    DeltaYijOldPair[atomIDj][atomIDi] = 0.0;
00191     }
00192    }
00193   }
00194  }
00195 }
00196
00197
00198
```

3.32 source/ComputePairForce.h File Reference

This graph shows which files directly or indirectly include this file:



Functions

- void ComputePairForce (int normFlag)

3.32.1 Function Documentation

3.32.1.1 ComputePairForce()

```
void ComputePairForce (
            int normFlag )
```

Definition at line 27 of file ComputePairForce.c.

```
00027                                {
00028 double dr[NDIM+1], fcVal, rr, ri, r, uVal;
00029 int n, i,j;
00030 uVal = 0.0;  uSumPair = 0.0 ;
00031 virSumPair = 0.0; virSumPairxx = 0.0; virSumPairyy = 0.0; virSumPairxy = 0.0;
00032
00033 for(n = 1 ; n <= nAtom ; n ++){
00034  ax[n] = 0.0;
00035  ay[n] = 0.0;
00036  discDragx[n] = 0.0;
00037  discDragy[n] = 0.0;
00038 }
00039 for(n = 1; n <= nPairTotal; n ++){
00040  PairID[n] = 0;
00041  Pairatom1[n] = 0;
00042  Pairatom2[n] = 0;
00043  PairXij[n] = 0.0;
00044  PairYij[n] = 0.0;
00045 }
00046
00047
00048 Kn = 1.0;
00049 double vr[NDIM+1], fdVal, rri;
00050 nPairActive = 0;
00051 double meff;
00052 meff = 0.0;
00053 int atomIDi, atomIDj;
00054 //int processThisPair = 1;
00055
00056 for(i=1;i<=nAtomInterface;i++){
00057  for(j=i+1;j<=nAtomInterface;j++){
00058   atomIDi = atomIDInterface[i];
00059   atomIDj = atomIDInterface[j];
00060   if (isBonded[atomIDi][atomIDj] == 0) { //To exclude pair interaction between bonded atoms
00061   rr = 0.0; rri = 0.0; fcVal = 0.0;  fdVal = 0.0; strech = 0.0;
00062   RadiusIJ = 0.0;
00063
00064   dr[1] = rx[atomIDi] - rx[atomIDj];
00065   if(dr[1] >= regionH[1])
00066    dr[1] -= region[1];
00067   else if(dr[1] < -regionH[1])
00068     dr[1] += region[1];
00069
00070   dr[2] = ry[atomIDi] - ry[atomIDj];
00071    if(dr[2] >= regionH[2]){
00072     dr[1] -= shearDisplacement;
00073     if(dr[1] < -regionH[1]) dr[1] += region[1];
00074     dr[2] -= region[2];
00075   }else if(dr[2] < -regionH[2]){
00076    dr[1] += shearDisplacement;
00077     if(dr[1] >= regionH[1]) dr[1] -= region[1];
00078    dr[2] += region[2];
00079   }
00080
00081   rr = Sqr(dr[1]) + Sqr(dr[2]);
00082   RadiusIJ = atomRadius[atomIDi] + atomRadius[atomIDj];
00083   SqrRadiusIJ = Sqr(RadiusIJ);
00084   if(rr < SqrRadiusIJ){
00085    r = sqrt(rr);
00086    ri = 1.0/r;
00087    rri = 1.0/rr;
00088    RadiusIJInv = 1.0/RadiusIJ;
00089    strech = (RadiusIJ - r);
00090    uVal = 0.5 * Kn * Sqr(strech);
00091
00092    //NormFlag
```

```
00093     if(normFlag == 1){
00094      strech = strech * RadiusIJInv;
00095      uVal = 0.5 * Kn * RadiusIJ * Sqr(strech);
00096      }
00097
00098     fcVal = Kn * strech * ri;
00099     vr[1] = vx[atomIDi] - vx[atomIDj];
00100     vr[2] = vy[atomIDi] - vy[atomIDj];
00101
00102     nPairActive++;
00103     PairID[nPairActive] = nPairActive;
00104     Pairatom1[nPairActive] = atomIDi;
00105     Pairatom2[nPairActive] = atomIDj;
00106     PairXij[nPairActive] = dr[1];
00107     PairYij[nPairActive] = dr[2];
00108
00109     //DampFlag = 1
00110     if(DampFlag == 1){
00111     meff = (atomMass[atomIDi]*atomMass[atomIDj])/(atomMass[atomIDi] + atomMass[atomIDj]);
00112     fdVal = -gamman * meff * (vr[1]*dr[1] + vr[2]*dr[2]) * rri; //disc-disc drag
00113
00114     discDragx[atomIDi] =  fdVal * dr[1]; //disc-disc drag
00115     discDragy[atomIDi] =  fdVal * dr[2]; //disc-disc drag
00116     discDragx[atomIDj] = -fdVal * dr[1]; //disc-disc drag
00117     discDragy[atomIDj] = -fdVal * dr[2]; //disc-disc drag
00118
00119     discDragx[nPairActive] = discDragx[atomIDi];
00120     discDragy[nPairActive] = discDragy[atomIDi];
00121
00122
00123     ax[atomIDi] += (fcVal + fdVal) * dr[1];
00124     ay[atomIDi] += (fcVal + fdVal) * dr[2];
00125     ax[atomIDj] += -(fcVal + fdVal) * dr[1];
00126     ay[atomIDj] += -(fcVal + fdVal) * dr[2];
00127    }
00128
00129    //DampFlag = 2
00130    else if(DampFlag == 2){
00131     discDragx[atomIDi] =  -gamman * vr[1]; //disc-disc drag
00132     discDragy[atomIDi] =  -gamman * vr[2]; //disc-disc drag
00133     discDragx[atomIDj] = -(-gamman * vr[1]); //disc-disc drag
00134     discDragy[atomIDj] = -(-gamman * vr[2]); //disc-disc drag
00135
00136     discDragx[nPairActive] = discDragx[atomIDi];
00137     discDragy[nPairActive] = discDragy[atomIDi];
00138
00139
00140     ax[atomIDi] +=  (fcVal * dr[1] - gamman * vr[1]);
00141     ay[atomIDi] +=  (fcVal * dr[2] - gamman * vr[2]);
00142     ax[atomIDj] += -(fcVal * dr[1] - gamman * vr[1]);
00143     ay[atomIDj] += -(fcVal * dr[2] - gamman * vr[2]);
00144    }
00145
00146    //DampFlag = 3. Suzanne PRL, 130, 178203 (2023) version
00147    else if(DampFlag == 3){
00148    //Track compression velocity
00149    DeltaXijNew = dr[1];
00150    DeltaYijNew = dr[2];
00151    if(stepCount == 0) { // Initialization step
00152     DeltaXijOldPair[atomIDi][atomIDj] = DeltaXijNew;
00153     DeltaYijOldPair[atomIDi][atomIDj] = DeltaYijNew;
00154     }
00155
00156     DeltaXij = DeltaXijNew - DeltaXijOldPair[atomIDi][atomIDj];
00157     DeltaYij = DeltaYijNew - DeltaYijOldPair[atomIDi][atomIDj];
00158     DeltaVXij = DeltaXij / deltaT;
00159     DeltaVYij = DeltaYij / deltaT;
00160
00161     // Update history for next step
00162     DeltaXijOldPair[atomIDi][atomIDj] = DeltaXijNew;
00163     DeltaYijOldPair[atomIDi][atomIDj] = DeltaYijNew;
00164
00165     discDragx[atomIDi] =  -gamman * DeltaVXij; //disc-disc drag
00166     discDragy[atomIDi] =  -gamman * DeltaVYij; //disc-disc drag
00167     discDragx[atomIDj] = -(-gamman * DeltaVXij); //disc-disc drag
00168     discDragy[atomIDj] = -(-gamman * DeltaVYij); //disc-disc drag
00169
00170     discDragx[nPairActive] = discDragx[atomIDi];
00171     discDragy[nPairActive] = discDragy[atomIDi];
00172
00173     ax[atomIDi] +=  (fcVal * dr[1] - gamman * DeltaVXij);
00174     ay[atomIDi] +=  (fcVal * dr[2] - gamman * DeltaVYij);
00175     ax[atomIDj] += -(fcVal * dr[1] - gamman * DeltaVXij);
00176     ay[atomIDj] += -(fcVal * dr[2] - gamman * DeltaVYij);
00177    }
00178
00179    //In the following, for stress/virial term (fcVal + fdVal) is used since the total pair force =
```

```
      Hookean Interaction + relative velocity drag
00180   uSumPair +=  0.5 * uVal;
00181   virSumPair += 0.5 * (fcVal + fdVal) * rr;
00182   virSumPairxx += 0.5 * (fcVal + fdVal) * dr[1] * dr[1];
00183   virSumPairyy += 0.5 * (fcVal + fdVal) * dr[2] * dr[2];
00184   virSumPairxy += 0.5 * (fcVal + fdVal) * dr[1] * dr[2];
00185     }
00186   else { //Resetting the distance between two discs when they are not in contact
00187    DeltaXijOldPair[atomIDi][atomIDj] = 0.0;
00188    DeltaYijOldPair[atomIDi][atomIDj] = 0.0;
00189    DeltaXijOldPair[atomIDj][atomIDi] = 0.0;
00190    DeltaYijOldPair[atomIDj][atomIDi] = 0.0;
00191     }
00192    }
00193   }
00194  }
00195 }
```

References atomIDInterface, atomMass, atomRadius, ax, ay, DampFlag, deltaT, DeltaVXij, DeltaVYij, DeltaXij, DeltaXijNew, DeltaXijOldPair, DeltaYij, DeltaYijNew, DeltaYijOldPair, discDragx, discDragy, gamman, isBonded, Kn, nAtom, nAtomInterface, NDIM, nPairActive, nPairTotal, Pairatom1, Pairatom2, PairID, PairXij, PairYij, RadiusIJ, RadiusIJInv, region, regionH, rx, ry, shearDisplacement, Sqr, SqrRadiusIJ, stepCount, strech, uSumPair, virSumPair, virSumPairxx, virSumPairxy, virSumPairyy, vx, and vy.

Referenced by main().

Here is the caller graph for this function:

3.33 ComputePairForce.h

Go to the documentation of this file.

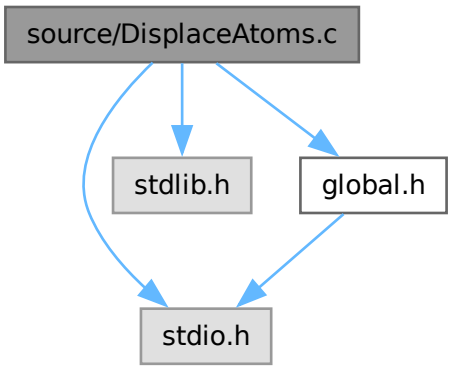
```
00001 #ifndef COMPUTE_PAIR_FORCE_H
00002 #define COMPUTE_PAIR_FORCE_H
00003
00004 void ComputePairForce(int normFlag);
00005
00006 #endif
00007
```

3.34 source/DisplaceAtoms.c File Reference

```
#include <stdio.h>
#include <stdlib.h>
```

```
#include "global.h"
```

Include dependency graph for DisplaceAtoms.c:



Functions

- void DisplaceAtoms ()

3.34.1 Function Documentation

3.34.1.1 DisplaceAtoms()

```
void DisplaceAtoms ( )
```

Definition at line 25 of file DisplaceAtoms.c.

```
00025                       {
00026  int n;
00027   for(n = 1; n <= nAtom; n ++){
00028    if(molID[n] == 2){
00029     rx[n] += DeltaX;
00030     ry[n] += DeltaY;
00031 } } }
```

References DeltaX, DeltaY, molID, nAtom, rx, and ry.

Referenced by main().

Here is the caller graph for this function:

3.35 DisplaceAtoms.c

Go to the documentation of this file.

```
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00007  * (at your option) any later version.
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00009  * Lamina is distributed in the hope that it will be useful,
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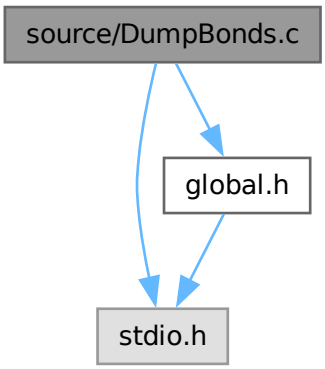
00016
00017  Copyright (C) 2025 Harish Charan, University of Durham, UK
00018
00019  */
00020
00021 #include<stdio.h>
00022 #include<stdlib.h>
00023 #include"global.h"
00024
00025 void DisplaceAtoms(){
00026  int n;
00027   for(n = 1; n <= nAtom; n ++){
00028    if(molID[n] == 2){
00029     rx[n] += DeltaX;
00030     ry[n] += DeltaY;
00031 } } }
```

3.36 source/DumpBonds.c File Reference

```
#include <stdio.h>
#include "global.h"
```

Include dependency graph for DumpBonds.c:



Functions

- void DumpBonds ()

3.36.1 Function Documentation

3.36.1.1 DumpBonds()

```
void DumpBonds ( )
```

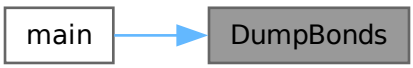
Definition at line 24 of file DumpBonds.c.

```
00024                {
00025   int n;
00026   //Trajectory file in LAMMPS dump format for OVITO visualization
00027   fprintf(fpbond, "ITEM: TIMESTEP\n");
00028   fprintf(fpbond, "%lf\n",timeNow);
00029   fprintf(fpbond, "ITEM: NUMBER OF ENTRIES\n");
00030   fprintf(fpbond, "%d\n",nBond);
00031   fprintf(fpbond, "ITEM: BOX BOUNDS pp ff pp\n");
00032   fprintf(fpbond, "%lf %lf xlo xhi\n", -regionH[1], regionH[1]);
00033   fprintf(fpbond, "%lf %lf ylo yhi\n", -regionH[2], regionH[2]);
00034   fprintf(fpbond, "%lf %lf zlo zhi\n", -0.1, 0.1);
00035   fprintf(fpbond, "ITEM: ENTRIES BondID, BondType, atom1 atom2 BondLength BondLengthEqul nodeDragx1
      nodeDragy1\n");
00036
00037   for(n=1; n<=nBond; n++)
00038    fprintf(fpbond, "%d %d %d %d %0.16lf %0.16lf %0.16lf %0.16lf\n", BondID[n], BondType[n], atom1[n],
      atom2[n],
00039    BondLength[n], ro[n], nodeDragx[atom1[n]], nodeDragy[atom1[n]]);
00040   }
```

References atom1, atom2, BondID, BondLength, BondType, fpbond, nBond, nodeDragx, nodeDragy, regionH, ro, and timeNow.

Referenced by main().

Here is the caller graph for this function:



3.37 DumpBonds.c

Go to the documentation of this file.

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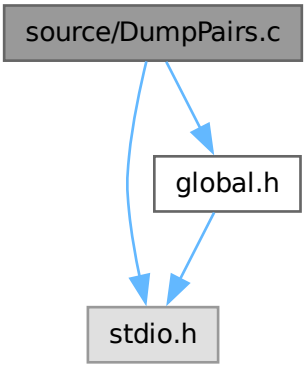
00016
00017  Copyright (C) 2025 Harish Charan, University of Durham, UK
00018
00019  */
00020
00021 #include<stdio.h>
```

```
00022 #include"global.h"
00023
00024 void DumpBonds(){
00025   int n;
00026   //Trajectory file in LAMMPS dump format for OVITO visualization
00027   fprintf(fpbond, "ITEM: TIMESTEP\n");
00028   fprintf(fpbond, "%lf\n",timeNow);
00029   fprintf(fpbond, "ITEM: NUMBER OF ENTRIES\n");
00030   fprintf(fpbond, "%d\n",nBond);
00031   fprintf(fpbond, "ITEM: BOX BOUNDS pp ff pp\n");
00032   fprintf(fpbond, "%lf %lf xlo xhi\n", -regionH[1], regionH[1]);
00033   fprintf(fpbond, "%lf %lf ylo yhi\n", -regionH[2], regionH[2]);
00034   fprintf(fpbond, "%lf %lf zlo zhi\n", -0.1, 0.1);
00035   fprintf(fpbond, "ITEM: ENTRIES BondID, BondType, atom1 atom2 BondLength BondLengthEqul nodeDragx1
      nodeDragy1\n");
00036
00037   for(n=1; n<=nBond; n++)
00038    fprintf(fpbond, "%d %d %d %d %0.16lf %0.16lf %0.16lf %0.16lf\n", BondID[n], BondType[n], atom1[n],
      atom2[n],
00039    BondLength[n], ro[n], nodeDragx[atom1[n]], nodeDragy[atom1[n]]);
00040   }
00041
00042
00043
```

3.38 source/DumpPairs.c File Reference

`#include <stdio.h>`
`#include "global.h"`
Include dependency graph for DumpPairs.c:



Functions

- void DumpPairs ()

3.38.1 Function Documentation

3.38.1.1 DumpPairs()

`void DumpPairs ( )`

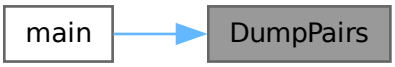
Definition at line 25 of file DumpPairs.c.

```
00025                 {
00026   int n;
00027   //Trajectory file in LAMMPS dump format for OVITO visualization
00028   fprintf(fppair, "ITEM: TIMESTEP\n");
00029   fprintf(fppair, "%lf\n",timeNow);
00030   fprintf(fppair, "ITEM: NUMBER OF ENTRIES\n");
00031   fprintf(fppair, "%d\n",nPairActive);
00032   fprintf(fppair, "ITEM: BOX BOUNDS pp ff pp\n");
00033   fprintf(fppair, "%lf %lf xlo xhi\n", -regionH[1], regionH[1]);
00034   fprintf(fppair, "%lf %lf ylo yhi\n", -regionH[2], regionH[2]);
00035   fprintf(fppair, "%lf %lf zlo zhi\n", -0.1, 0.1);
00036   fprintf(fppair, "ITEM: ENTRIES index, atom1 atom2 xij yij discDragx1 discDragy1\n");
00037
00038   for(n=1; n<=nPairActive; n++)
00039    fprintf(fppair, "%d %d %d %0.16lf %0.16lf %0.16lf %0.16lf\n", PairID[n], Pairatom1[n],
      Pairatom2[n],
00040    PairXij[n], PairYij[n], discDragx[n], discDragy[n]);
00041
00042   }
```

References discDragx, discDragy, fppair, nPairActive, Pairatom1, Pairatom2, PairID, PairXij, PairYij, regionH, and timeNow.

Referenced by main().

Here is the caller graph for this function:



3.39 DumpPairs.c

Go to the documentation of this file.

```
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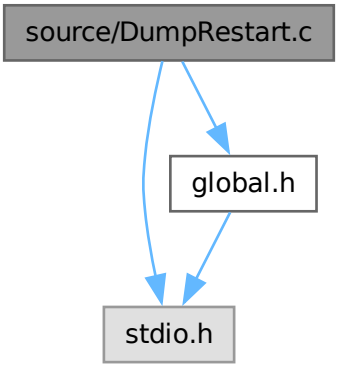
00016
00017  Copyright (C) 2025 Harish Charan, University of Durham, UK
00018
00019  */
00020
00021
00022 #include<stdio.h>
00023 #include"global.h"
00024
00025 void DumpPairs(){
00026   int n;
00027   //Trajectory file in LAMMPS dump format for OVITO visualization
00028   fprintf(fppair, "ITEM: TIMESTEP\n");
00029   fprintf(fppair, "%lf\n",timeNow);
00030   fprintf(fppair, "ITEM: NUMBER OF ENTRIES\n");
00031   fprintf(fppair, "%d\n",nPairActive);
```

```
00032   fprintf(fppair, "ITEM: BOX BOUNDS pp ff pp\n");
00033   fprintf(fppair, "%lf %lf xlo xhi\n", -regionH[1], regionH[1]);
00034   fprintf(fppair, "%lf %lf ylo yhi\n", -regionH[2], regionH[2]);
00035   fprintf(fppair, "%lf %lf zlo zhi\n", -0.1, 0.1);
00036   fprintf(fppair, "ITEM: ENTRIES index, atom1 atom2 xij yij discDragx1 discDragy1\n");
00037
00038   for(n=1; n<=nPairActive; n++)
00039    fprintf(fppair, "%d %d %d %0.16lf %0.16lf %0.16lf %0.16lf\n", PairID[n], Pairatom1[n],
      Pairatom2[n],
00040    PairXij[n], PairYij[n], discDragx[n], discDragy[n]);
00041
00042   }
00043
00044
00045
```

3.40 source/DumpRestart.c File Reference

```
#include <stdio.h>
#include "global.h"
```

Include dependency graph for DumpRestart.c:



Functions

- void DumpRestart ()

3.40.1 Function Documentation

3.40.1.1 DumpRestart()

```
void DumpRestart ( )
```

Definition at line 25 of file DumpRestart.c.

```
00025                   {
00026  char DUMP[256];
00027  FILE *fpDUMP;
00028  sprintf(DUMP, "%s.Restart", prefix);
00029  fpDUMP = fopen(DUMP, "w");
00030  if(fpDUMP == NULL) {
```

```
00031   fprintf(stderr, "Error opening file %s for writing\n", DUMP);
00032   return;
00033  }
00034
00035   fprintf(fpDUMP, "timeNow %lf\n", timeNow);
00036   fprintf(fpDUMP, "nAtom %d\n",  nAtom);
00037   fprintf(fpDUMP, "nBond %d\n", nBond);
00038   fprintf(fpDUMP, "nAtomType %d\n", nAtomType);
00039   fprintf(fpDUMP, "nBondType %d\n", nBondType);
00040   fprintf(fpDUMP, "region[1] %0.14lf\n", region[1]);
00041   fprintf(fpDUMP, "region[2] %0.14lf\n", region[2]);
00042
00043   int n;
00044   fprintf(fpDUMP, "Atoms\n");
00045   for(n = 1; n <= nAtom; n ++)
00046    fprintf(fpDUMP, "%d %d %d %0.2lf %0.16lf %0.16lf %0.16lf %0.16lf\n", atomID[n], molID[n],
      atomType[n], atomRadius[n], rx[n], ry[n], vx[n], vy[n]);
00047
00048
00049   fprintf(fpDUMP, "Bonds\n");
00050   for(n=1; n<=nBond; n++)
00051   fprintf(fpDUMP,  "%d %d %d %d %0.2lf %0.16lf\n", BondID[n], BondType[n], atom1[n], atom2[n], kb[n],
      ro[n]);
00052
00053   fclose(fpDUMP);
00054 }
```

References atom1, atom2, atomID, atomRadius, atomType, BondID, BondType, kb, molID, nAtom, nAtomType, nBond, nBondType, prefix, region, ro, rx, ry, timeNow, vx, and vy.

Referenced by main().

Here is the caller graph for this function:

3.41 DumpRestart.c

Go to the documentation of this file.

```
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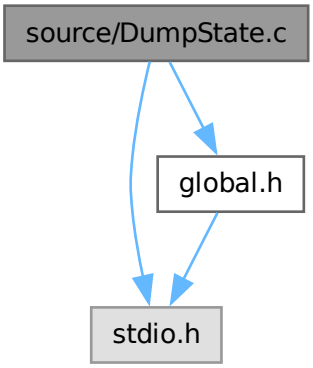
00015  * along with Lamina. If not, see <https://www.gnu.org/licenses/>.
00016
00017  Copyright (C) 2025 Harish Charan, University of Durham, UK
00018
00019  */
00020
00021
00022 #include <stdio.h>
00023 #include "global.h"
00024
00025 void DumpRestart() {
```

```
00026  char DUMP[256];
00027  FILE *fpDUMP;
00028  sprintf(DUMP, "%s.Restart", prefix);
00029  fpDUMP = fopen(DUMP, "w");
00030  if(fpDUMP == NULL) {
00031   fprintf(stderr, "Error opening file %s for writing\n", DUMP);
00032   return;
00033  }
00034
00035   fprintf(fpDUMP, "timeNow %lf\n", timeNow);
00036   fprintf(fpDUMP, "nAtom %d\n",  nAtom);
00037   fprintf(fpDUMP, "nBond %d\n", nBond);
00038   fprintf(fpDUMP, "nAtomType %d\n", nAtomType);
00039   fprintf(fpDUMP, "nBondType %d\n", nBondType);
00040   fprintf(fpDUMP, "region[1] %0.14lf\n", region[1]);
00041   fprintf(fpDUMP, "region[2] %0.14lf\n", region[2]);
00042
00043   int n;
00044   fprintf(fpDUMP, "Atoms\n");
00045   for(n = 1; n <= nAtom; n ++)
00046    fprintf(fpDUMP, "%d %d %d %0.2lf %0.16lf %0.16lf %0.16lf %0.16lf\n", atomID[n], molID[n],
      atomType[n], atomRadius[n], rx[n], ry[n], vx[n], vy[n]);
00047
00048
00049   fprintf(fpDUMP, "Bonds\n");
00050   for(n=1; n<=nBond; n++)
00051   fprintf(fpDUMP,  "%d %d %d %d %0.2lf %0.16lf\n", BondID[n], BondType[n], atom1[n], atom2[n], kb[n],
      ro[n]);
00052
00053   fclose(fpDUMP);
00054 }
00055
```

3.42 source/DumpState.c File Reference

```
#include <stdio.h>
#include "global.h"
```

Include dependency graph for DumpState.c:



Functions

- void DumpState ()

3.42.1 Function Documentation

3.42.1.1 DumpState()

```
void DumpState ( )
```

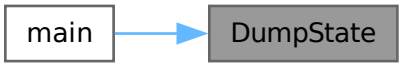
Definition at line 25 of file DumpState.c.

```
00025                   {
00026  char DUMP[256];
00027  FILE *fpDUMP;
00028  sprintf(DUMP, "%s.STATE", prefix);
00029  fpDUMP = fopen(DUMP, "w");
00030  if(fpDUMP == NULL) {
00031   fprintf(stderr, "Error opening file %s for writing\n", DUMP);
00032   return;
00033  }
00034
00035   fprintf(fpDUMP, "ITEM: TIMESTEP\n");
00036   fprintf(fpDUMP, "%lf\n",timeNow);
00037   fprintf(fpDUMP, "ITEM: NUMBER OF ATOMS\n");
00038   fprintf(fpDUMP, "%d\n",nAtom);
00039   fprintf(fpDUMP, "ITEM: BOX BOUNDS pp pp pp\n");
00040   fprintf(fpDUMP, "%lf %lf xlo xhi\n", -regionH[1], regionH[1]);
00041   fprintf(fpDUMP, "%lf %lf ylo yhi\n", -regionH[2], regionH[2]);
00042   fprintf(fpDUMP, "%lf %lf zlo zhi\n",  -0.1, 0.1);
00043   fprintf(fpDUMP, "ITEM: ATOMS id mol type radius x y vx vy fx fy\n");
00044   int n;
00045   for (n = 1; n <= nAtom; n++) {
00046    fprintf(fpDUMP, "%d\t %d\t %d\t %0.21f\t %0.16lf\t %0.16lf\t %0.16lf\t %0.16lf\t %0.16lf\t
      %0.16lf\n",
00047    atomID[n], molID[n], atomType[n], atomRadius[n], rx[n], ry[n], vx[n], vy[n], ax[n], ay[n]);
00048   }
00049   fclose(fpDUMP);
00050 }
```

References atomID, atomRadius, atomType, ax, ay, molID, nAtom, prefix, regionH, rx, ry, timeNow, vx, and vy.

Referenced by main().

Here is the caller graph for this function:



3.43 DumpState.c

Go to the documentation of this file.

```
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00011  * MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the
00012  * GNU General Public License for more details.
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```

```
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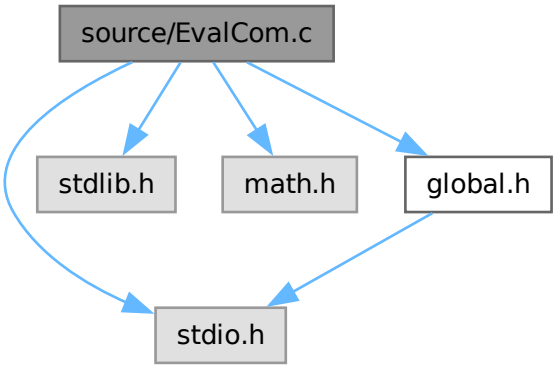
00016
00017  Copyright (C) 2025 Harish Charan, University of Durham, UK
00018
00019  */
00020
00021
00022 #include <stdio.h>
00023 #include "global.h"
00024
00025 void DumpState() {
00026  char DUMP[256];
00027  FILE *fpDUMP;
00028  sprintf(DUMP, "%s.STATE", prefix);
00029  fpDUMP = fopen(DUMP, "w");
00030  if(fpDUMP == NULL) {
00031   fprintf(stderr, "Error opening file %s for writing\n", DUMP);
00032   return;
00033  }
00034
00035   fprintf(fpDUMP, "ITEM: TIMESTEP\n");
00036   fprintf(fpDUMP, "%lf\n",timeNow);
00037   fprintf(fpDUMP, "ITEM: NUMBER OF ATOMS\n");
00038   fprintf(fpDUMP, "%d\n",nAtom);
00039   fprintf(fpDUMP, "ITEM: BOX BOUNDS pp pp pp\n");
00040   fprintf(fpDUMP, "%lf %lf xlo xhi\n", -regionH[1], regionH[1]);
00041   fprintf(fpDUMP, "%lf %lf ylo yhi\n", -regionH[2], regionH[2]);
00042   fprintf(fpDUMP, "%lf %lf zlo zhi\n",  -0.1, 0.1);
00043   fprintf(fpDUMP, "ITEM: ATOMS id mol type radius x y vx vy fx fy\n");
00044   int n;
00045   for (n = 1; n <= nAtom; n++) {
00046    fprintf(fpDUMP, "%d\t %d\t %d\t %0.2lf\t %0.16lf\t %0.16lf\t %0.16lf\t %0.16lf\t %0.16lf\t
      %0.16lf\n",
00047    atomID[n], molID[n], atomType[n], atomRadius[n], rx[n], ry[n], vx[n], vy[n], ax[n], ay[n]);
00048   }
00049   fclose(fpDUMP);
00050 }
00051
```

3.44 source/EvalCom.c File Reference

```
#include <stdio.h>
#include <stdlib.h>
#include <math.h>
#include "global.h"
```

Include dependency graph for EvalCom.c:



Functions

- void EvalCom ()

3.44.1 Function Documentation

3.44.1.1 EvalCom()

```
void EvalCom ( )
```

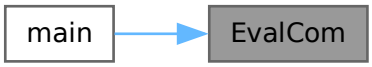
Definition at line 27 of file EvalCom.c.

```
00027                {
00028  int n;
00029  ComX = 0.0; ComY = 0.0; ComXRatio = 0.0; ComYRatio = 0.0;
00030  TotalMass = 0.0;
00031
00032  for(n=1; n<=nAtom; n++){
00033  if(molID[n] == 2){
00034   ComX += atomMass[n] * rxUnwrap[n];
00035   ComY += atomMass[n] * ryUnwrap[n];
00036   TotalMass += atomMass[n];
00037   } }
00038
00039   ComX = ComX/TotalMass;
00040   ComY = ComY/TotalMass;
00041
00042   if(timeNow == 0.0){
00043   ComX0 = ComX; ComY0 = ComY;
00044   }
00045   ComXRatio = ComX/ComX0;    ComYRatio = ComY/ComY0;
00046  }
```

References atomMass, ComX, ComX0, ComXRatio, ComY, ComY0, ComYRatio, molID, nAtom, rxUnwrap, ryUnwrap, timeNow, and TotalMass.

Referenced by main().

Here is the caller graph for this function:



3.45 EvalCom.c

Go to the documentation of this file.

```
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00008  *
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```

```
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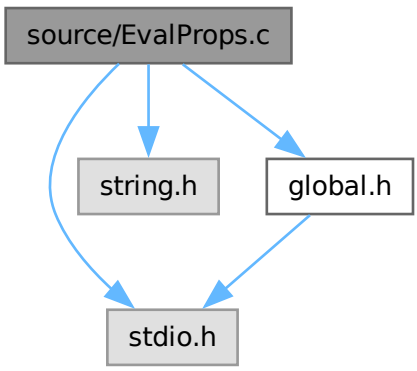
00015  * along with Lamina. If not, see <https://www.gnu.org/licenses/>.
00016
00017  Copyright (C) 2025 Harish Charan, University of Durham, UK
00018
00019  */
00020
00021
00022 #include<stdio.h>
00023 #include<stdlib.h>
00024 #include<math.h>
00025 #include"global.h"
00026
00027 void EvalCom(){
00028  int n;
00029  ComX = 0.0; ComY = 0.0; ComXRatio = 0.0; ComYRatio = 0.0;
00030  TotalMass = 0.0;
00031
00032  for(n=1; n<=nAtom; n++){
00033  if(molID[n] == 2){
00034   ComX += atomMass[n] * rxUnwrap[n];
00035   ComY += atomMass[n] * ryUnwrap[n];
00036   TotalMass += atomMass[n];
00037   } }
00038
00039   ComX = ComX/TotalMass;
00040   ComY = ComY/TotalMass;
00041
00042   if(timeNow == 0.0){
00043   ComX0 = ComX; ComY0 = ComY;
00044   }
00045   ComXRatio = ComX/ComX0;    ComYRatio = ComY/ComY0;
00046  }
00047
00048
00049
```

3.46 source/EvalProps.c File Reference

```
#include <stdio.h>
#include <string.h>
#include "global.h"
```

Include dependency graph for EvalProps.c:



Functions

- void EvalProps ()

3.46.1 Function Documentation

3.46.1.1 EvalProps()

```
void EvalProps ( )
```

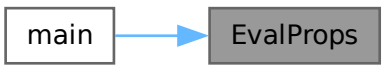
Definition at line 26 of file EvalProps.c.

```
00026                 {
00027  real v, vv;
00028  virSum = 0.0;
00029  vSumX = 0.0; vSumY = 0.0; vSum = 0.0;
00030  vvSum = 0.;
00031  int n;
00032
00033  for (n = 1; n <= nAtom; n++) {
00034   vv = 0.;
00035   // Initialize v with a default value to avoid "uninitialized" warning.
00036   v = 0.0;
00037   // X direction velocity
00038   if (strcmp(solver, "Verlet") == 0) {
00039     v = vx[n];
00040   } else if (strcmp(solver, "LeapFrog") == 0) {
00041     v = vx[n] - 0.5 * deltaT * ax[n];
00042   }
00043    vSum += v;
00044    vv += Sqr(v);
00045    vSumX += v;
00046    // Y direction velocity
00047    if (strcmp(solver, "Verlet") == 0) {
00048    v = vy[n];
00049    } else if (strcmp(solver, "LeapFrog") == 0) {
00050    v = vy[n] - 0.5 * deltaT * ay[n];
00051    }
00052    vSum += v;
00053    vSumY += v;
00054    vv += Sqr(v);
00055    vvSum += vv;
00056   }
00057
00058   kinEnergy = 0.5 * vvSum / nAtom ;
00059   uSumPairPerAtom = uSumPair / nAtom ;
00060   BondEnergyPerAtom = TotalBondEnergy / (0.5*nAtom); //Factor of 0.5 since each atom has one half the
      bond energy
00061   potEnergy = uSumPairPerAtom +  BondEnergyPerAtom ;
00062   totEnergy = kinEnergy + potEnergy;
00063   virSumxx = virSumPairxx  + virSumBondxx ;
00064   virSumyy = virSumPairyy  + virSumBondyy ;
00065   virSumxy = virSumPairxy  + virSumBondxy ;
00066   virSum = virSumPair + virSumBond;
00067   pressure = density * (vvSum + virSum) / (nAtom * NDIM);
00068
00069 }
```

References ax, ay, BondEnergyPerAtom, deltaT, density, kinEnergy, nAtom, NDIM, potEnergy, pressure, solver, Sqr, TotalBondEnergy, totEnergy, uSumPair, uSumPairPerAtom, virSum, virSumBond, virSumBondxx, virSumBondxy, virSumBondyy, virSumPair, virSumPairxx, virSumPairxy, virSumPairyy, virSumxx, virSumxy, virSumyy, vSum, vSumX, vSumY, vvSum, vx, and vy.

Referenced by main().

Here is the caller graph for this function:



3.47 EvalProps.c

Go to the documentation of this file.

```
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00009  * Lamina is distributed in the hope that it will be useful,
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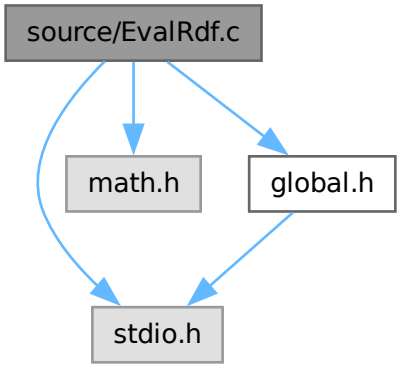
00016
00017  Copyright (C) 2025 Harish Charan, University of Durham, UK
00018
00019  */
00020
00021
00022 #include <stdio.h>
00023 #include <string.h>
00024 #include "global.h"
00025
00026 void EvalProps() {
00027  real v, vv;
00028  virSum = 0.0;
00029  vSumX = 0.0; vSumY = 0.0; vSum = 0.0;
00030  vvSum = 0.;
00031  int n;
00032
00033  for (n = 1; n <= nAtom; n++) {
00034   vv = 0.;
00035   // Initialize v with a default value to avoid "uninitialized" warning.
00036   v = 0.0;
00037   // X direction velocity
00038   if (strcmp(solver, "Verlet") == 0) {
00039     v = vx[n];
00040   } else if (strcmp(solver, "LeapFrog") == 0) {
00041     v = vx[n] - 0.5 * deltaT * ax[n];
00042   }
00043    vSum += v;
00044    vv += Sqr(v);
00045    vSumX += v;
00046    // Y direction velocity
00047    if (strcmp(solver, "Verlet") == 0) {
00048    v = vy[n];
00049    } else if (strcmp(solver, "LeapFrog") == 0) {
00050    v = vy[n] - 0.5 * deltaT * ay[n];
00051    }
00052    vSum += v;
00053    vSumY += v;
00054    vv += Sqr(v);
00055    vvSum += vv;
00056   }
00057
00058   kinEnergy = 0.5 * vvSum / nAtom ;
00059   uSumPairPerAtom = uSumPair / nAtom ;
00060   BondEnergyPerAtom = TotalBondEnergy / (0.5*nAtom); //Factor of 0.5 since each atom has one half the
      bond energy
00061   potEnergy = uSumPairPerAtom +  BondEnergyPerAtom ;
00062   totEnergy = kinEnergy + potEnergy;
00063   virSumxx = virSumPairxx  + virSumBondxx ;
00064   virSumyy = virSumPairyy  + virSumBondyy ;
00065   virSumxy = virSumPairxy  + virSumBondxy ;
00066   virSum = virSumPair + virSumBond;
00067   pressure = density * (vvSum + virSum) / (nAtom * NDIM);
00068
00069 }
00070
```

3.48 source/EvalRdf.c File Reference

```
#include <stdio.h>
#include <math.h>
```

```
#include "global.h"
```

Include dependency graph for EvalRdf.c:



Functions

- void EvalRdf ()

3.48.1 Function Documentation

3.48.1.1 EvalRdf()

```
void EvalRdf ( )
```

Definition at line 26 of file EvalRdf.c.

```
00026                {
00027   real dr[NDIM+1], deltaR, normFac, rr, rrRange;
00028   int j1, j2, n;
00029   countRdf ++;
00030   if(countRdf == 1){
00031     for(n = 1 ; n <= sizeHistRdf ; n ++)
00032       histRdf[n] = 0.;
00033   }
00034   rrRange = Sqr(rangeRdf);
00035   deltaR = rangeRdf / sizeHistRdf;
00036   for(j1 = 1 ; j1 <= nAtom - 1 ; j1 ++){
00037     for(j2 = j1 + 1 ; j2 <= nAtom ; j2 ++){
00038
00039       dr[1] = rx[j1] - rx[j2];
00040       if(fabs(dr[1]) > regionH[1])
00041     dr[1] -= SignR(region[1], dr[1]);
00042
00043       dr[2] = ry[j1] - ry[j2];
00044       if(fabs(dr[2]) > regionH[2])
00045     dr[2] -= SignR(region[2], dr[2]);
00046
00047       rr = Sqr(dr[1]) + Sqr(dr[2]);
00048
00049       if(rr < rrRange){
00050     n = (int)(sqrt(rr)/deltaR) + 1;
00051     histRdf[n] ++;
00052       }
00053     }
00054   }
00055
00056   if(countRdf == limitRdf){
```

```
00057     normFac = region[1]*region[2] / (M_PI*Sqr(deltaR)*nAtom*nAtom*countRdf );
00058     for(n = 1 ; n <= sizeHistRdf ; n ++)
00059       histRdf[n] *= normFac/(n-0.5);
00060     // PRINT THE RADIAL DISTRIBUTION DATA ON TO DISK FILE
00061     real rBin;
00062     int n;
00063     fprintf(fprdf,"rdf @ timeNow %lf\n", timeNow);
00064     for(n = 1 ; n <= sizeHistRdf ; n ++){
00065       rBin = (n - 0.5)*rangeRdf/sizeHistRdf;
00066       fprintf(fprdf, "%lf %lf\n", rBin, histRdf[n]);
00067     }
00068   }
00069
00070 }
```

References countRdf, fprdf, histRdf, limitRdf, nAtom, NDIM, rangeRdf, region, regionH, rx, ry, SignR, sizeHistRdf, Sqr, and timeNow.

3.49 EvalRdf.c

Go to the documentation of this file.

```
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00009  * Lamina is distributed in the hope that it will be useful,
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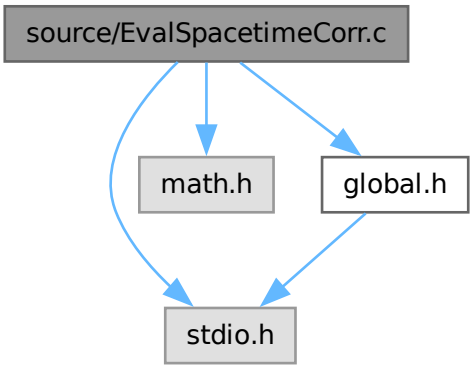
00016
00017  Copyright (C) 2025 Harish Charan, University of Durham, UK
00018
00019  */
00020
00021
00022 #include<stdio.h>
00023 #include<math.h>
00024 #include"global.h"
00025
00026 void EvalRdf(){
00027   real dr[NDIM+1], deltaR, normFac, rr, rrRange;
00028   int j1, j2, n;
00029   countRdf ++;
00030   if(countRdf == 1){
00031     for(n = 1 ; n <= sizeHistRdf ; n ++)
00032       histRdf[n] = 0.;
00033   }
00034   rrRange = Sqr(rangeRdf);
00035   deltaR = rangeRdf / sizeHistRdf;
00036   for(j1 = 1 ; j1 <= nAtom - 1 ; j1 ++){
00037     for(j2 = j1 + 1 ; j2 <= nAtom ; j2 ++){
00038
00039       dr[1] = rx[j1] - rx[j2];
00040       if(fabs(dr[1]) > regionH[1])
00041     dr[1] -= SignR(region[1], dr[1]);
00042
00043       dr[2] = ry[j1] - ry[j2];
00044       if(fabs(dr[2]) > regionH[2])
00045     dr[2] -= SignR(region[2], dr[2]);
00046
00047       rr = Sqr(dr[1]) + Sqr(dr[2]);
00048
00049       if(rr < rrRange){
00050     n = (int)(sqrt(rr)/deltaR) + 1;
00051     histRdf[n] ++;
00052       }
00053     }
00054   }
00055
00056   if(countRdf == limitRdf){
00057     normFac = region[1]*region[2] / (M_PI*Sqr(deltaR)*nAtom*nAtom*countRdf );
00058     for(n = 1 ; n <= sizeHistRdf ; n ++)
00059       histRdf[n] *= normFac/(n-0.5);
```

```
00060     // PRINT THE RADIAL DISTRIBUTION DATA ON TO DISK FILE
00061     real rBin;
00062     int n;
00063     fprintf(fprdf,"rdf @ timeNow %lf\n", timeNow);
00064     for(n = 1 ; n <= sizeHistRdf ; n ++){
00065       rBin = (n - 0.5)*rangeRdf/sizeHistRdf;
00066       fprintf(fprdf, "%lf %lf\n", rBin, histRdf[n]);
00067     }
00068   }
00069
00070 }
00071
```

3.50 source/EvalSpacetimeCorr.c File Reference

```
#include <stdio.h>
#include <math.h>
#include "global.h"
```

Include dependency graph for EvalSpacetimeCorr.c:



Functions

- void EvalSpacetimeCorr ()

3.50.1 Function Documentation

3.50.1.1 EvalSpacetimeCorr()

```
void EvalSpacetimeCorr ( )
```

Definition at line 26 of file EvalSpacetimeCorr.c.

```
00026                          {
00027   real cosV=0., cosV0=0., cosV1=0., cosV2=0., sinV=0., sinV1=0., sinV2=0.;
00028   real COSA, SINA, COSV, SINV;
00029   int j, m, n, nb, ni, nv;
00030   real kMin = 2. * M_PI / region[1];
00031   real kMax = M_PI;
00032   real deltaK = (kMax - kMin) / nFunCorr;
```

```
00033
00034   for (j = 1; j <= 2*nFunCorr; j++)
00035     cfVal[j] = 0.;
00036
00037   for (n = 1; n <= nAtom; n++){
00038     j = 1;
00039     COSA = cos(kMin*rx[n]);
00040     SINA = sin(kMin*rx[n]);
00041     for (m = 1; m <= nFunCorr; m++){
00042       if(m == 1){
00043     cosV = cos(deltaK*rx[n]);
00044     sinV = sin(deltaK*rx[n]);
00045     cosV0 = cosV;
00046       }else if(m == 2){
00047     cosV1 = cosV;
00048     sinV1 = sinV;
00049     cosV = 2.*cosV0*cosV1-1;
00050     sinV = 2.*cosV0*sinV1;
00051       }else{
00052     cosV2 = cosV1;
00053     sinV2 = sinV1;
00054     cosV1 = cosV;
00055     sinV1 = sinV;
00056     cosV = 2.*cosV0*cosV1-cosV2;
00057     sinV = 2.*cosV0*sinV1-sinV2;
00058       }
00059       COSV = COSA*cosV - SINA*sinV;
00060       SINV = SINA*cosV + COSA*sinV;
00061       cfVal[j] += COSV;
00062       cfVal[j+1] += SINV;
00063       j += 2;
00064     }
00065   }
00066
00067   for (nb = 1; nb <= nBuffCorr; nb++){
00068     indexCorr[nb] += 1;
00069     if (indexCorr[nb] <= 0) continue;
00070     ni = nFunCorr * (indexCorr[nb] - 1);
00071     if (indexCorr[nb] == 1){
00072       for (j = 1; j <= 2*nFunCorr; j++)
00073     cfOrg[nb][j] = cfVal[j];
00074     }
00075
00076     for (j = 1; j <= nFunCorr; j++)
00077       spacetimeCorr[nb][ni + j] = 0.;
00078
00079     j = 1;
00080     for (m = 1; m <= nFunCorr; m++){
00081       nv = m + ni;
00082       spacetimeCorr[nb][nv] += cfVal[j] * cfOrg[nb][j] + cfVal[j + 1] * cfOrg[nb][j + 1];
00083       j += 2;
00084     }
00085
00086   }
00087
00088   // ACCUMULATE SPACETIME CORRELATIONS
00089   for (nb = 1; nb <= nBuffCorr; nb++){
00090    if (indexCorr[nb] == nValCorr){
00091      for (j = 1; j <= nFunCorr*nValCorr; j++)
00092        spacetimeCorrAv[j] += spacetimeCorr[nb][j];
00093     indexCorr[nb] = 0.;
00094     countCorrAv ++;
00095     if (countCorrAv == limitCorrAv){
00096       for (j = 1; j <= nFunCorr*nValCorr; j++)
00097     spacetimeCorrAv[j] /= (nAtom*limitCorrAv);
00098       fprintf(fpdnsty,"NDIM %d\n", NDIM);
00099       fprintf(fpdnsty,"nAtom %d\n", nAtom);
00100       fprintf(fpdnsty,"region %lf\n", region[1]);
00101       fprintf(fpdnsty,"nFunCorr %d\n", nFunCorr);
00102       fprintf(fpdnsty,"limitCorrAv %d\n", limitCorrAv);
00103       fprintf(fpdnsty,"stepCorr %d\n", stepCorr);
00104       fprintf(fpdnsty,"nValCorr %d\n", nValCorr);
00105       fprintf(fpdnsty,"deltaT %lf\n", deltaT);
00106       real tVal;
00107       for (n = 1; n <= nValCorr; n++){
00108     tVal = (n-1)*stepCorr*deltaT;
00109     fprintf (fpdnsty, "%e\t", tVal);
00110     int nn = nFunCorr*(n-1);
00111     for (j = 1; j <= nFunCorr; j ++)
00112           fprintf (fpdnsty, "%e\t", spacetimeCorrAv[nn + j]);
00113         fprintf (fpdnsty, "\n");
00114       }
00115
00116       countCorrAv = 0.;
00117       for (j = 1; j <= nFunCorr*nValCorr; j++)
00118     spacetimeCorrAv[j] = 0.;
00119     }
```

```
00120     }
00121   }
00122 }
```

References cfOrg, cfVal, countCorrAv, deltaT, fpdnsty, indexCorr, limitCorrAv, nAtom, nBuffCorr, NDIM, nFunCorr, nValCorr, region, rx, spacetimeCorr, spacetimeCorrAv, and stepCorr.

3.51 EvalSpacetimeCorr.c

Go to the documentation of this file.

```
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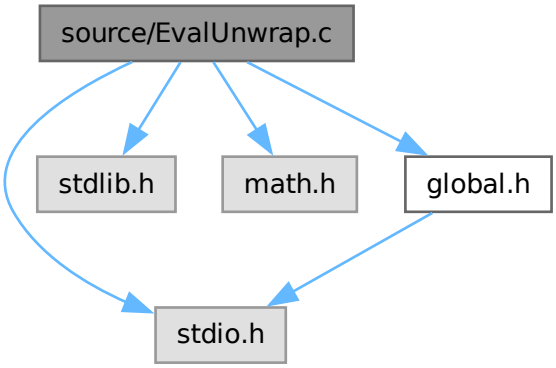
00016
00017  Copyright (C) 2025 Harish Charan, University of Durham, UK
00018
00019  */
00020
00021
00022 #include<stdio.h>
00023 #include<math.h>
00024 #include"global.h"
00025
00026 void EvalSpacetimeCorr (){
00027   real cosV=0., cosV0=0., cosV1=0., cosV2=0., sinV=0., sinV1=0., sinV2=0.;
00028   real COSA, SINA, COSV, SINV;
00029   int j, m, n, nb, ni, nv;
00030   real kMin = 2. * M_PI / region[1];
00031   real kMax = M_PI;
00032   real deltaK = (kMax - kMin) / nFunCorr;
00033
00034   for (j = 1; j <= 2*nFunCorr; j++)
00035     cfVal[j] = 0.;
00036
00037   for (n = 1; n <= nAtom; n++){
00038     j = 1;
00039     COSA = cos(kMin*rx[n]);
00040     SINA = sin(kMin*rx[n]);
00041     for (m = 1; m <= nFunCorr; m++){
00042       if(m == 1){
00043     cosV = cos(deltaK*rx[n]);
00044     sinV = sin(deltaK*rx[n]);
00045     cosV0 = cosV;
00046       }else if(m == 2){
00047     cosV1 = cosV;
00048     sinV1 = sinV;
00049     cosV = 2.*cosV0*cosV1-1;
00050     sinV = 2.*cosV0*sinV1;
00051       }else{
00052     cosV2 = cosV1;
00053     sinV2 = sinV1;
00054     cosV1 = cosV;
00055     sinV1 = sinV;
00056     cosV = 2.*cosV0*cosV1-cosV2;
00057     sinV = 2.*cosV0*sinV1-sinV2;
00058       }
00059       COSV = COSA*cosV - SINA*sinV;
00060       SINV = SINA*cosV + COSA*sinV;
00061       cfVal[j] += COSV;
00062       cfVal[j+1] += SINV;
00063       j += 2;
00064     }
00065   }
00066
00067   for (nb = 1; nb <= nBuffCorr; nb++){
00068     indexCorr[nb] += 1;
00069     if (indexCorr[nb] <= 0) continue;
00070     ni = nFunCorr * (indexCorr[nb] - 1);
```

```
00071     if (indexCorr[nb] == 1){
00072       for (j = 1; j <= 2*nFunCorr; j++)
00073     cfOrg[nb][j] = cfVal[j];
00074     }
00075
00076     for (j = 1; j <= nFunCorr; j++)
00077       spacetimeCorr[nb][ni + j] = 0.;
00078
00079     j = 1;
00080     for (m = 1; m <= nFunCorr; m++){
00081       nv = m + ni;
00082       spacetimeCorr[nb][nv] += cfVal[j] * cfOrg[nb][j] + cfVal[j + 1] * cfOrg[nb][j + 1];
00083       j += 2;
00084     }
00085
00086   }
00087
00088   // ACCUMULATE SPACETIME CORRELATIONS
00089   for (nb = 1; nb <= nBuffCorr; nb++){
00090    if (indexCorr[nb] == nValCorr){
00091      for (j = 1; j <= nFunCorr*nValCorr; j++)
00092        spacetimeCorrAv[j] += spacetimeCorr[nb][j];
00093      indexCorr[nb] = 0.;
00094      countCorrAv ++;
00095      if (countCorrAv == limitCorrAv){
00096        for (j = 1; j <= nFunCorr*nValCorr; j++)
00097      spacetimeCorrAv[j] /= (nAtom*limitCorrAv);
00098        fprintf(fpdnsty,"NDIM %d\n", NDIM);
00099        fprintf(fpdnsty,"nAtom %d\n", nAtom);
00100        fprintf(fpdnsty,"region %lf\n", region[1]);
00101        fprintf(fpdnsty,"nFunCorr %d\n", nFunCorr);
00102        fprintf(fpdnsty,"limitCorrAv %d\n", limitCorrAv);
00103        fprintf(fpdnsty,"stepCorr %d\n", stepCorr);
00104        fprintf(fpdnsty,"nValCorr %d\n", nValCorr);
00105        fprintf(fpdnsty,"deltaT %lf\n", deltaT);
00106        real tVal;
00107        for (n = 1; n <= nValCorr; n++){
00108      tVal = (n-1)*stepCorr*deltaT;
00109      fprintf (fpdnsty, "%e\t", tVal);
00110      int nn = nFunCorr*(n-1);
00111      for (j = 1; j <= nFunCorr; j ++)
00112            fprintf (fpdnsty, "%e\t", spacetimeCorrAv[nn + j]);
00113          fprintf (fpdnsty, "\n");
00114        }
00115
00116        countCorrAv = 0.;
00117        for (j = 1; j <= nFunCorr*nValCorr; j++)
00118      spacetimeCorrAv[j] = 0.;
00119      }
00120    }
00121   }
00122 }
```

3.52 source/EvalUnwrap.c File Reference

```
#include <stdio.h>
#include <stdlib.h>
#include <math.h>
#include "global.h"
```

Include dependency graph for EvalUnwrap.c:



Functions

- void EvalUnwrap ()

3.52.1 Function Documentation

3.52.1.1 EvalUnwrap()

```
void EvalUnwrap ( )
```

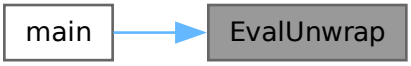
Definition at line 27 of file EvalUnwrap.c.

```
00027                   {
00028  int n;
00029  for (n = 1; n <= nAtom; n++) {
00030   rxUnwrap[n] = rx[n] + ImageX[n] * region[1];
00031   ryUnwrap[n] = ry[n] + ImageY[n] * region[2];
00032   }
00033 }
```

References ImageX, ImageY, nAtom, region, rx, rxUnwrap, ry, and ryUnwrap.

Referenced by main().

Here is the caller graph for this function:



3.53 EvalUnwrap.c

Go to the documentation of this file.

```
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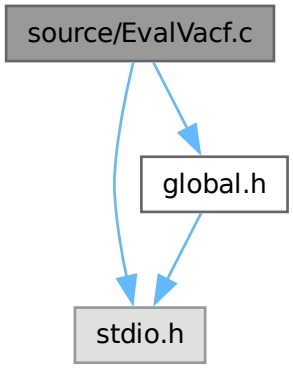
00016
00017  Copyright (C) 2025 Harish Charan, University of Durham, UK
00018
00019  */
00020
00021
00022 #include <stdio.h>
00023 #include <stdlib.h>
00024 #include <math.h>
00025 #include "global.h"
00026
00027 void EvalUnwrap() {
00028  int n;
00029  for (n = 1; n <= nAtom; n++) {
00030   rxUnwrap[n] = rx[n] + ImageX[n] * region[1];
00031   ryUnwrap[n] = ry[n] + ImageY[n] * region[2];
00032   }
00033 }
00034
```

3.54 source/EvalVacf.c File Reference

```
#include <stdio.h>
#include "global.h"
```

Include dependency graph for EvalVacf.c:



Functions

- void AccumVacf ()
- void EvalVacf ()

3.54.1 Function Documentation

3.54.1.1 AccumVacf()

```
void AccumVacf ( )
```

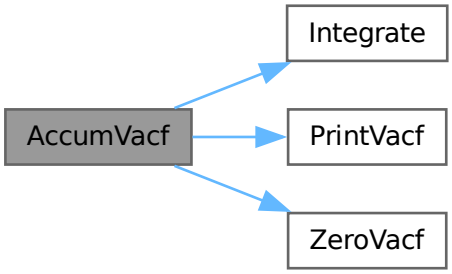
Definition at line 27 of file AccumVacf.c.

```
00027                   {
00028  double fac;
00029  int j, nb;
00030  for(nb = 1 ; nb <= nBuffAcf ; nb ++){
00031   if(indexAcf[nb] == nValAcf){
00032    for(j = 1 ; j <= nValAcf; j ++){
00033     viscAcfAv[j] +=  viscAcf[nb][j];
00034     }
00035   indexAcf[nb] = 0;
00036   countAcfAv ++;
00037   if(countAcfAv == limitAcfAv){
00038    fac = 1./(kinEnergy*region[1]*region[2]*limitAcfAv);
00039    viscAcfInt = fac*stepAcf*deltaT*Integrate(viscAcfAv, nValAcf);
00040    PrintVacf();
00041    ZeroVacf();
00042 } } } }
```

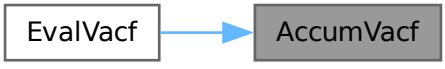
References countAcfAv, deltaT, indexAcf, Integrate(), kinEnergy, limitAcfAv, nBuffAcf, nValAcf, PrintVacf(), region, stepAcf, viscAcf, viscAcfAv, viscAcfInt, and ZeroVacf().

Referenced by EvalVacf().

Here is the call graph for this function:



Here is the caller graph for this function:



3.54.1.2 EvalVacf()

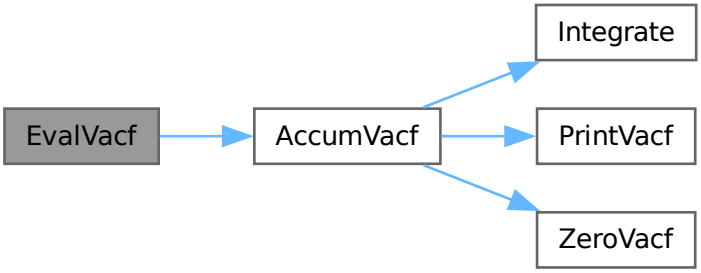
```
void EvalVacf ( )
```

Definition at line 26 of file EvalVacf.c.

```
00026                {
00027   int n, nb, ni;
00028   double viscVec = 0.;
00029   double v[3];
00030   for(n = 1 ; n <= nAtom ; n ++){
00031     v[1] = vx[n] - 0.5*ax[n]*deltaT;
00032     v[2] = vy[n] - 0.5*ay[n]*deltaT;
00033     viscVec += v[1]*v[2];
00034   }
00035   viscVec += rfAtom;
00036   for(nb = 1 ; nb <= nBuffAcf ; nb ++){
00037     indexAcf[nb] ++;
00038     if(indexAcf[nb] <= 0)continue;
00039     if(indexAcf[nb] == 1){
00040       viscAcfOrg[nb] = viscVec;
00041     }
00042     ni = indexAcf[nb];
00043     viscAcf[nb][ni] = viscAcfOrg[nb]*viscVec;
00044   }
00045   AccumVacf();
00046 }
```

References AccumVacf(), ax, ay, deltaT, indexAcf, nAtom, nBuffAcf, rfAtom, viscAcf, viscAcfOrg, vx, and vy.

Here is the call graph for this function:



3.55 EvalVacf.c

Go to the documentation of this file.

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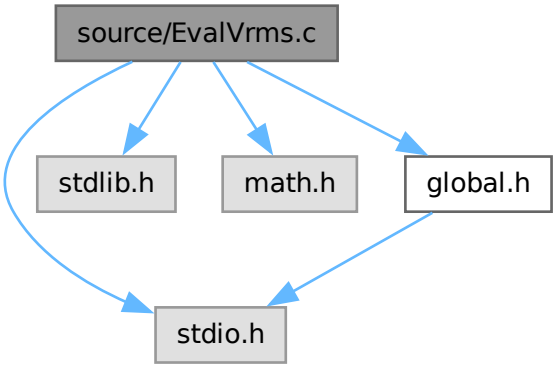
00016
00017  Copyright (C) 2025 Harish Charan, University of Durham, UK
```

```
00018
00019  */
00020
00021
00022 #include<stdio.h>
00023 #include"global.h"
00024
00025 void AccumVacf();
00026 void EvalVacf(){
00027   int n, nb, ni;
00028   double viscVec = 0.;
00029   double v[3];
00030   for(n = 1 ; n <= nAtom ; n ++){
00031     v[1] = vx[n] - 0.5*ax[n]*deltaT;
00032     v[2] = vy[n] - 0.5*ay[n]*deltaT;
00033     viscVec += v[1]*v[2];
00034   }
00035   viscVec += rfAtom;
00036   for(nb = 1 ; nb <= nBuffAcf ; nb ++){
00037     indexAcf[nb] ++;
00038     if(indexAcf[nb] <= 0)continue;
00039     if(indexAcf[nb] == 1){
00040       viscAcfOrg[nb] = viscVec;
00041     }
00042     ni = indexAcf[nb];
00043     viscAcf[nb][ni] = viscAcfOrg[nb]*viscVec;
00044   }
00045   AccumVacf();
00046 }
```

3.56 source/EvalVrms.c File Reference

```
#include <stdio.h>
#include <stdlib.h>
#include <math.h>
#include "global.h"
```

Include dependency graph for EvalVrms.c:



Functions

- void EvalVrms ()

3.56.1 Function Documentation

3.56.1.1 EvalVrms()

```
void EvalVrms ( )
```

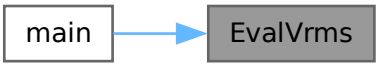
Definition at line 27 of file EvalVrms.c.

```
00027                {
00028   int n;
00029   VSqr = 0.0;
00030   VMeanSqr = 0.0;
00031   VRootMeanSqr = 0.0;
00032
00033   for(n = 1 ; n <= nAtom ; n ++){
00034   VSqr += Sqr(vx[n]) + Sqr(vy[n]);
00035   }
00036   VMeanSqr = VSqr/nAtom;
00037   VRootMeanSqr = sqrt(VMeanSqr);
00038   }
```

References nAtom, Sqr, VMeanSqr, VRootMeanSqr, VSqr, vx, and vy.

Referenced by main().

Here is the caller graph for this function:



3.57 EvalVrms.c

Go to the documentation of this file.

```
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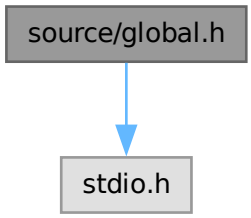
00017  Copyright (C) 2025 Harish Charan, University of Durham, UK
00018
00019  */
00020
00021
00022 #include<stdio.h>
00023 #include<stdlib.h>
00024 #include<math.h>
00025 #include"global.h"
00026
00027 void EvalVrms(){
00028   int n;
00029   VSqr = 0.0;
```

```
00030   VMeanSqr = 0.0;
00031   VRootMeanSqr = 0.0;
00032
00033   for(n = 1 ; n <= nAtom ; n ++){
00034   VSqr += Sqr(vx[n]) + Sqr(vy[n]);
00035   }
00036   VMeanSqr = VSqr/nAtom;
00037   VRootMeanSqr = sqrt(VMeanSqr);
00038   }
00039
00040
00041
```

3.58 source/global.h File Reference

`#include <stdio.h>`
Include dependency graph for global.h:



This graph shows which files directly or indirectly include this file:

Macros

- #define EXTERN extern
- #define NDIM 2
- #define Sqr(x) ((x) ∗ (x))
- #define SignR(x, y) (((y) >= 0) ? (x) : (- (x)))

Typedefs

- typedef double real

Variables

- double * rx
- double * ry
- double * vx
- double * vy
- double * ax
- double * ay
- double * speed
- double region [2+1]
- double regionH [2+1]
- double deltaT
- double timeNow
- double potEnergy
- double kinEnergy
- double totEnergy
- double density
- double pressure
- double rCut
- double kappa
- double uSum
- double virSum
- double svirSum
- double vSum
- double vSumX
- double vSumY
- double vvSum
- double sPotEnergy
- double sKinEnergy
- double sTotEnergy
- double sPressure
- double ssPotEnergy
- double ssKinEnergy
- double ssTotEnergy
- double ssPressure
- int initUcell [2+1]
- int moreCycles
- int nAtom
- int stepAvg
- int stepCount
- int stepEquil
- int stepLimit
- int stepTraj
- int stepDump
- double RadiusIJ
- double SqrRadiusIJ
- double RadiusIJInv
- int nAtomType
- int * atomType
- int * atomID
- double * atomRadius
- double * atomMass
- double TotalMass
- int nBond
- int nBondType

- int * atom1
- int * atom2
- int * BondID
- int * BondType
- double * kb
- double * ro
- double * BondEnergy
- double * BondLength
- double TotalBondEnergy
- double BondEnergyPerAtom
- double gamman
- double * discDragx
- double * discDragy
- double * nodeDragx
- double * nodeDragy
- double strain
- double strainRate
- double shearDisplacement
- double shearVelocity
- double VSqr
- double VMeanSqr
- double VRootMeanSqr
- double ComX
- double ComY
- double ComX0
- double ComY0
- double ComXRatio
- double ComYRatio
- double HaltCondition
- double DeltaY
- double DeltaX
- int * ImageX
- int * ImageY
- double * rxUnwrap
- double * ryUnwrap
- int nAtomInterface
- int nDiscInterface
- int nAtomBlock
- int * atomIDInterface
- double Kn
- double fx
- double fy
- double FyByIx
- double fxByfy
- int DampFlag
- double strech
- int dumpPairFlag
- int nPairTotal
- int nPairActive
- int * PairID
- int * Pairatom1
- int * Pairatom2
- double * PairXij
- double * PairYij
- char solver [128]

- char xBoundary [10]
- char yBoundary [10]
- char thermo
- double * DeltaXijOld
- double * DeltaYijOld
- double DeltaXijNew
- double DeltaYijNew
- double DeltaXij
- double DeltaYij
- double DeltaVXij
- double DeltaVYij
- double ** DeltaXijOldPair
- double ** DeltaYijOldPair
- int * molID
- int ** isBonded
- int * cellList
- int cells [2+1]
- int rank
- int size
- int master
- double * fax
- double * fay
- double fuSum
- double fvirSum
- double frfAtom
- double uSumPair
- double uSumPairPerAtom
- double virSumPair
- double virSumPairxx
- double virSumPairyy
- double virSumPairxy
- double virSumBond
- double virSumBondxx
- double virSumBondyy
- double virSumBondxy
- double virSumxx
- double virSumyy
- double virSumxy
- int freezeAtomType
- double ** cfOrg
- double ** spacetimeCorr
- double * cfVal
- double * spacetimeCorrAv
- int * indexCorr
- int countCorrAv
- int limitCorrAv
- int nBuffCorr
- int nFunCorr
- int nValCorr
- int stepCorr
- double rfAtom
- double * indexAcf
- double ** viscAcf
- double * viscAcfOrg
- double * viscAcfAv

- double viscAcfInt
- int nValAcf
- int nBuffAcf
- int stepAcf
- int countAcfAv
- int limitAcfAv
- double * histRdf
- double rangeRdf
- int countRdf
- int limitRdf
- int sizeHistRdf
- int stepRdf
- char * prefix
- char result [250]
- FILE * fpresult
- char xyz [256]
- FILE * fpxyz
- char bond [256]
- FILE * fpbond
- char dump [256]
- FILE * fpdump
- char dnsty [256]
- FILE * fpdnsty
- char visc [256]
- FILE * fpvisc
- char rdf [256]
- FILE * fprdf
- char vrms [256]
- FILE * fpvrms
- char stress [256]
- FILE * fpstress
- char momentum [256]
- FILE * fpmomentum
- char com [256]
- FILE * fpcom
- char pair [256]
- FILE * fppair

3.58.1 Macro Definition Documentation

3.58.1.1 EXTERN

```
#define EXTERN extern
```

Definition at line 8 of file global.h.

3.58.1.2 NDIM

```
#define NDIM 2
```

Definition at line 13 of file global.h.

Referenced by ComputeBondForce(), ComputeForcesCells(), ComputePairForce(), EvalProps(), EvalRdf(), EvalSpacetimeCorr(), and LeapfrogStep().

3.58.1.3 SignR

```
#define SignR(
              x,
              y ) (((y) >= 0) ?  (x) :  (- (x)))
```

Definition at line 15 of file global.h.

Referenced by EvalRdf(), and LeapfrogStep().

3.58.1.4 Sqr

```
#define Sqr(
              x ) ((x) * (x))
```

Definition at line 14 of file global.h.

Referenced by AccumProps(), BrownianStep(), ComputeBondForce(), ComputeForcesCells(), ComputePairForce(), EvalProps(), EvalRdf(), EvalVrms(), and LeapfrogStep().

3.58.2 Typedef Documentation

3.58.2.1 real

```
typedef double real
```

Definition at line 11 of file global.h.

3.58.3 Variable Documentation

3.58.3.1 atom1

```
int* atom1  [extern]
```

Referenced by Close(), ComputeBondForce(), DumpBonds(), DumpRestart(), and Init().

3.58.3.2 atom2

```
int * atom2
```

Definition at line 34 of file global.h.

Referenced by Close(), ComputeBondForce(), DumpBonds(), DumpRestart(), and Init().

3.58.3.3 atomID

```
int* atomID  [extern]
```

Referenced by Close(), DumpRestart(), DumpState(), Init(), and Trajectory().

3.58.3.4 atomIDInterface

```
int* atomIDInterface  [extern]
```

Referenced by Close(), ComputePairForce(), and Init().

3.58.3.5 atomMass

```
double* atomMass  [extern]
```

Referenced by Close(), ComputePairForce(), EvalCom(), and Init().

3.58.3.6 atomRadius

```
double* atomRadius  [extern]
```

Referenced by ApplyBoundaryCond(), Close(), ComputeForcesCells(), ComputePairForce(), DumpRestart(), DumpState(), Init(), and Trajectory().

3.58.3.7 atomType

```
int* atomType  [extern]
```

Referenced by ApplyDrivingForce(), Close(), DumpRestart(), DumpState(), Init(), Trajectory(), and VelocityVerletStep().

3.58.3.8 ax

```
double * ax
```

Definition at line 17 of file global.h.

Referenced by ApplyDrivingForce(), ApplyForce(), ApplyViscous(), BrownianStep(), Close(), ComputeBondForce(), ComputeForcesCells(), ComputePairForce(), DumpState(), EvalProps(), EvalVacf(), Init(), LeapfrogStep(), Trajectory(), and VelocityVerletStep().

3.58.3.9 ay

```
double * ay
```

Definition at line 17 of file global.h.

Referenced by ApplyDrivingForce(), ApplyForce(), ApplyViscous(), BrownianStep(), Close(), ComputeBondForce(), ComputeForcesCells(), ComputePairForce(), DumpState(), EvalProps(), EvalVacf(), Init(), LeapfrogStep(), Trajectory(), and VelocityVerletStep().

3.58.3.10 bond

```
char bond[256]  [extern]
```

Referenced by main().

3.58.3.11 BondEnergy

```
double* BondEnergy  [extern]
```

Referenced by ComputeBondForce(), and Init().

3.58.3.12 BondEnergyPerAtom

```
double BondEnergyPerAtom
```

Definition at line 38 of file global.h.

Referenced by EvalProps(), and PrintSummary().

3.58.3.13 BondID

```
int* BondID  [extern]
```

Referenced by Close(), DumpBonds(), DumpRestart(), and Init().

3.58.3.14 BondLength

```
double * BondLength
```

Definition at line 37 of file global.h.

Referenced by ComputeBondForce(), DumpBonds(), and Init().

3.58.3.15 BondType

```
int * BondType
```

Definition at line 35 of file global.h.

Referenced by Close(), DumpBonds(), DumpRestart(), and Init().

3.58.3.16 cellList

```
int* cellList  [extern]
```

Referenced by Close(), ComputeForcesCells(), and Init().

3.58.3.17 cells

```
int cells[2+1]
```

Definition at line 78 of file global.h.

Referenced by ComputeForcesCells(), and Init().

3.58.3.18 cfOrg

```
double** cfOrg  [extern]
```

Referenced by AllocArrays(), Close(), and EvalSpacetimeCorr().

3.58.3.19 cfVal

```
double * cfVal
```

Definition at line 89 of file global.h.

Referenced by AllocArrays(), Close(), and EvalSpacetimeCorr().

3.58.3.20 com

```
char com[256]  [extern]
```

Referenced by main().

3.58.3.21 ComX

```
double ComX  [extern]
```

Referenced by EvalCom(), and PrintCom().

3.58.3.22 ComX0

```
double ComX0
```

Definition at line 44 of file global.h.

Referenced by EvalCom().

3.58.3.23 ComXRatio

```
double ComXRatio
```

Definition at line 44 of file global.h.

Referenced by EvalCom().

3.58.3.24 ComY

```
double ComY
```

Definition at line 44 of file global.h.

Referenced by EvalCom(), and PrintCom().

3.58.3.25 ComY0

```
double ComY0
```

Definition at line 44 of file global.h.

Referenced by EvalCom().

3.58.3.26 ComYRatio

```
double ComYRatio
```

Definition at line 44 of file global.h.

Referenced by EvalCom().

3.58.3.27 countAcfAv

```
int countAcfAv
```

Definition at line 95 of file global.h.

Referenced by AccumVacf(), and ZeroVacf().

3.58.3.28 countCorrAv

```
int countCorrAv
```

Definition at line 90 of file global.h.

Referenced by EvalSpacetimeCorr(), and SetupJob().

3.58.3.29 countRdf

```
int countRdf  [extern]
```

Referenced by EvalRdf(), and SetupJob().

3.58.3.30 DampFlag

```
int DampFlag  [extern]
```

Referenced by ComputeBondForce(), ComputePairForce(), and Init().

3.58.3.31 deltaT

```
double deltaT
```

Definition at line 20 of file global.h.

Referenced by AccumVacf(), BrownianStep(), ComputeBondForce(), ComputePairForce(), EvalProps(), EvalSpacetimeCorr(), EvalVacf(), Init(), LeapfrogStep(), main(), PrintVacf(), and VelocityVerletStep().

3.58.3.32 DeltaVXij

```
double DeltaVXij
```

Definition at line 70 of file global.h.

Referenced by ComputeBondForce(), and ComputePairForce().

3.58.3.33 DeltaVYij

```
double DeltaVYij
```

Definition at line 70 of file global.h.

Referenced by ComputeBondForce(), and ComputePairForce().

3.58.3.34 DeltaX

```
double DeltaX
```

Definition at line 46 of file global.h.

Referenced by DisplaceAtoms(), and Init().

3.58.3.35 DeltaXij

```
double DeltaXij  [extern]
```

Referenced by ComputeBondForce(), and ComputePairForce().

3.58.3.36 DeltaXijNew

```
double DeltaXijNew  [extern]
```

Referenced by ComputeBondForce(), and ComputePairForce().

3.58.3.37 DeltaXijOld

```
double* DeltaXijOld  [extern]
```

Referenced by Close(), ComputeBondForce(), and Init().

3.58.3.38 DeltaXijOldPair

```
double** DeltaXijOldPair  [extern]
```

Referenced by Close(), ComputePairForce(), and Init().

3.58.3.39 DeltaY

```
double DeltaY  [extern]
```

Referenced by DisplaceAtoms(), and Init().

3.58.3.40 DeltaYij

```
double DeltaYij
```

Definition at line 70 of file global.h.

Referenced by ComputeBondForce(), and ComputePairForce().

3.58.3.41 DeltaYijNew

```
double DeltaYijNew
```

Definition at line 69 of file global.h.

Referenced by ComputeBondForce(), and ComputePairForce().

3.58.3.42 DeltaYijOld

```
double * DeltaYijOld
```

Definition at line 68 of file global.h.

Referenced by Close(), ComputeBondForce(), and Init().

3.58.3.43 DeltaYijOldPair

```
double ** DeltaYijOldPair
```

Definition at line 71 of file global.h.

Referenced by Close(), ComputePairForce(), and Init().

3.58.3.44 density

```
double density
```

Definition at line 21 of file global.h.

Referenced by EvalProps(), and Init().

3.58.3.45 discDragx

```
double* discDragx  [extern]
```

Referenced by ComputeForcesCells(), ComputePairForce(), DumpPairs(), and Init().

3.58.3.46 discDragy

```
double * discDragy
```

Definition at line 40 of file global.h.

Referenced by ComputeForcesCells(), ComputePairForce(), DumpPairs(), and Init().

3.58.3.47 dnsty

```
char dnsty[256]  [extern]
```

3.58.3.48 dump

```
char dump[256]  [extern]
```

3.58.3.49 dumpPairFlag

```
int dumpPairFlag  [extern]
```

3.58.3.50 fax

```
double* fax  [extern]
```

Referenced by Close(), and Init().

3.58.3.51 fay

```
double * fay
```

Definition at line 80 of file global.h.

Referenced by Close(), and Init().

3.58.3.52 fpbond

```
FILE* fpbond  [extern]
```

Referenced by DumpBonds(), and main().

3.58.3.53 fpcom

```
FILE* fpcom  [extern]
```

Referenced by Init(), main(), and PrintCom().

3.58.3.54 fpdnsty

```
FILE* fpdnsty  [extern]
```

Referenced by EvalSpacetimeCorr().

3.58.3.55 fpdump

```
FILE* fpdump  [extern]
```

3.58.3.56 fpmomentum

```
FILE* fpmomentum  [extern]
```

Referenced by PrintMomentum().

3.58.3.57 fppair

```
FILE* fppair  [extern]
```

Referenced by DumpPairs(), and main().

3.58.3.58 fprdf

```
FILE* fprdf  [extern]
```

Referenced by EvalRdf().

3.58.3.59 fpresult

```
FILE* fpresult  [extern]
```

Referenced by ApplyBoundaryCond(), HaltConditionCheck(), Init(), main(), and PrintSummary().

3.58.3.60 fpstress

```
FILE* fpstress  [extern]
```

Referenced by PrintStress().

3.58.3.61 fpvisc

```
FILE* fpvisc  [extern]
```

Referenced by PrintVacf().

3.58.3.62 fpvrms

```
FILE* fpvrms  [extern]
```

Referenced by Init(), main(), and PrintVrms().

3.58.3.63 fpxyz

```
FILE* fpxyz  [extern]
```

Referenced by main(), and Trajectory().

3.58.3.64 freezeAtomType

```
int freezeAtomType  [extern]
```

Referenced by Init(), and VelocityVerletStep().

3.58.3.65 frfAtom

```
double frfAtom
```

Definition at line 80 of file global.h.

3.58.3.66 fuSum

```
double fuSum
```

Definition at line 80 of file global.h.

3.58.3.67 fvirSum

```
double fvirSum
```

Definition at line 80 of file global.h.

3.58.3.68 fx

```
double fx  [extern]
```

Referenced by ApplyForce().

3.58.3.69 fxByfy

```
double fxByfy
```

Definition at line 52 of file global.h.

Referenced by ApplyForce(), and Init().

3.58.3.70 fy

```
double fy
```

Definition at line 52 of file global.h.

Referenced by ApplyForce().

3.58.3.71 FyBylx

```
double FyBylx
```

Definition at line 52 of file global.h.

Referenced by ApplyForce(), and Init().

3.58.3.72 gamman

```
double gamman  [extern]
```

Referenced by ComputeBondForce(), ComputeForcesCells(), ComputePairForce(), and Init().

3.58.3.73 HaltCondition

```
double HaltCondition  [extern]
```

Referenced by HaltConditionCheck(), and Init().

3.58.3.74 histRdf

```
double* histRdf  [extern]
```

Referenced by AllocArrays(), and EvalRdf().

3.58.3.75 ImageX

```
int* ImageX  [extern]
```

Referenced by Close(), EvalUnwrap(), Init(), and VelocityVerletStep().

3.58.3.76 ImageY

```
int * ImageY
```

Definition at line 47 of file global.h.

Referenced by Close(), EvalUnwrap(), Init(), and VelocityVerletStep().

3.58.3.77 indexAcf

```
double* indexAcf  [extern]
```

Referenced by AccumVacf(), AllocArrays(), Close(), EvalVacf(), and InitVacf().

3.58.3.78 indexCorr

```
int* indexCorr  [extern]
```

Referenced by AllocArrays(), Close(), EvalSpacetimeCorr(), and SetupJob().

3.58.3.79 initUcell

```
int initUcell[2+1]  [extern]
```

3.58.3.80 isBonded

```
int** isBonded  [extern]
```

Referenced by Close(), ComputePairForce(), and Init().

3.58.3.81 kappa

```
double kappa
```

Definition at line 21 of file global.h.

Referenced by Init(), and LeapfrogStep().

3.58.3.82 kb

```
double* kb  [extern]
```

Referenced by Close(), ComputeBondForce(), DumpRestart(), and Init().

3.58.3.83 kinEnergy

```
double kinEnergy
```

Definition at line 20 of file global.h.

Referenced by AccumProps(), AccumVacf(), EvalProps(), and PrintSummary().

3.58.3.84 Kn

```
double Kn  [extern]
```

Referenced by ComputePairForce().

3.58.3.85 limitAcfAv

```
int limitAcfAv
```

Definition at line 95 of file global.h.

Referenced by AccumVacf(), and Init().

3.58.3.86 limitCorrAv

```
int limitCorrAv
```

Definition at line 90 of file global.h.

Referenced by EvalSpacetimeCorr(), and Init().

3.58.3.87 limitRdf

```
int limitRdf
```

Definition at line 99 of file global.h.

Referenced by EvalRdf(), and Init().

3.58.3.88 master

```
int master
```

Definition at line 79 of file global.h.

3.58.3.89 molID

```
int* molID  [extern]
```

Referenced by ApplyForce(), Close(), DisplaceAtoms(), DumpRestart(), DumpState(), EvalCom(), Init(), and Trajectory().

3.58.3.90 momentum

```
char momentum[256]  [extern]
```

3.58.3.91 moreCycles

```
int moreCycles
```

Definition at line 24 of file global.h.

Referenced by main().

3.58.3.92 nAtom

```
int nAtom
```

Definition at line 24 of file global.h.

Referenced by ApplyBoundaryCond(), ApplyDrivingForce(), ApplyForce(), ApplyLeesEdwardsBoundaryCond(), ApplyShear(), ApplyViscous(), BrownianStep(), Close(), ComputeBondForce(), ComputeForcesCells(), ComputePairForce(), DisplaceAtoms(), DumpRestart(), DumpState(), EvalCom(), EvalProps(), EvalRdf(), EvalSpacetimeCorr(), EvalUnwrap(), EvalVacf(), EvalVrms(), Init(), LeapfrogStep(), Trajectory(), and VelocityVerletStep().

3.58.3.93 nAtomBlock

```
int nAtomBlock
```

Definition at line 49 of file global.h.

Referenced by ApplyForce(), and Init().

3.58.3.94 nAtomInterface

```
int nAtomInterface  [extern]
```

Referenced by ComputePairForce(), and Init().

3.58.3.95 nAtomType

```
int nAtomType  [extern]
```

Referenced by DumpRestart(), and Init().

3.58.3.96 nBond

```
int nBond  [extern]
```

Referenced by ComputeBondForce(), DumpBonds(), DumpRestart(), and Init().

3.58.3.97 nBondType

```
int nBondType
```

Definition at line 33 of file global.h.

Referenced by DumpRestart(), and Init().

3.58.3.98 nBuffAcf

```
int nBuffAcf
```

Definition at line 95 of file global.h.

Referenced by AccumVacf(), AllocArrays(), Close(), EvalVacf(), Init(), and InitVacf().

3.58.3.99 nBuffCorr

```
int nBuffCorr
```

Definition at line 90 of file global.h.

Referenced by AllocArrays(), Close(), EvalSpacetimeCorr(), Init(), and SetupJob().

3.58.3.100 nDiscInterface

```
int nDiscInterface
```

Definition at line 49 of file global.h.

Referenced by Init().

3.58.3.101 nFunCorr

```
int nFunCorr
```

Definition at line 90 of file global.h.

Referenced by AllocArrays(), EvalSpacetimeCorr(), Init(), and SetupJob().

3.58.3.102 nodeDragx

```
double * nodeDragx
```

Definition at line 40 of file global.h.

Referenced by ComputeBondForce(), DumpBonds(), and Init().

3.58.3.103 nodeDragy

```
double * nodeDragy
```

Definition at line 40 of file global.h.

Referenced by ComputeBondForce(), DumpBonds(), and Init().

3.58.3.104 nPairActive

```
int nPairActive
```

Definition at line 58 of file global.h.

Referenced by ComputePairForce(), and DumpPairs().

3.58.3.105 nPairTotal

```
int nPairTotal  [extern]
```

Referenced by ComputePairForce(), and Init().

3.58.3.106 nValAcf

```
int nValAcf  [extern]
```

Referenced by AccumVacf(), AllocArrays(), Init(), InitVacf(), PrintVacf(), and ZeroVacf().

3.58.3.107 nValCorr

```
int nValCorr
```

Definition at line 90 of file global.h.

Referenced by AllocArrays(), EvalSpacetimeCorr(), Init(), and SetupJob().

3.58.3.108 pair

```
char pair[256]  [extern]
```

Referenced by main().

3.58.3.109 Pairatom1

```
int * Pairatom1
```

Definition at line 59 of file global.h.

Referenced by Close(), ComputePairForce(), DumpPairs(), and Init().

3.58.3.110 Pairatom2

```
int * Pairatom2
```

Definition at line 59 of file global.h.

Referenced by Close(), ComputePairForce(), DumpPairs(), and Init().

3.58.3.111 PairID

```
int* PairID  [extern]
```

Referenced by Close(), ComputePairForce(), DumpPairs(), and Init().

3.58.3.112 PairXij

```
double* PairXij  [extern]
```

Referenced by Close(), ComputePairForce(), DumpPairs(), and Init().

3.58.3.113 PairYij

```
double * PairYij
```

Definition at line 60 of file global.h.

Referenced by Close(), ComputePairForce(), DumpPairs(), and Init().

3.58.3.114 potEnergy

```
double potEnergy
```

Definition at line 20 of file global.h.

Referenced by AccumProps(), EvalProps(), and PrintSummary().

3.58.3.115 prefix

```
char* prefix  [extern]
```

Definition at line 13 of file main.c.

Referenced by DumpRestart(), and DumpState().

3.58.3.116 pressure

```
double pressure
```

Definition at line 21 of file global.h.

Referenced by AccumProps(), EvalProps(), PrintStress(), and PrintSummary().

3.58.3.117 RadiusIJ

```
double RadiusIJ  [extern]
```

Referenced by ComputeForcesCells(), and ComputePairForce().

3.58.3.118 RadiusIJInv

```
double RadiusIJInv
```

Definition at line 26 of file global.h.

Referenced by ComputeForcesCells(), and ComputePairForce().

3.58.3.119 rangeRdf

```
double rangeRdf
```

Definition at line 98 of file global.h.

Referenced by EvalRdf(), and Init().

3.58.3.120 rank

```
int rank  [extern]
```

Referenced by ComputeForcesCells().

3.58.3.121 rCut

```
double rCut
```

Definition at line 21 of file global.h.

Referenced by Init(), and LeapfrogStep().

3.58.3.122 rdf

```
char rdf[256]  [extern]
```

3.58.3.123 region

```
double region[2+1]  [extern]
```

Referenced by AccumVacf(), ApplyBoundaryCond(), ApplyLeesEdwardsBoundaryCond(), ComputeBondForce(), ComputeForcesCells(), ComputePairForce(), DumpRestart(), EvalRdf(), EvalSpacetimeCorr(), EvalUnwrap(), Init(), LeapfrogStep(), and VelocityVerletStep().

3.58.3.124 regionH

```
double regionH[2+1]
```

Definition at line 20 of file global.h.

Referenced by ApplyBoundaryCond(), ApplyForce(), ApplyLeesEdwardsBoundaryCond(), ComputeBondForce(), ComputeForcesCells(), ComputePairForce(), DumpBonds(), DumpPairs(), DumpState(), EvalRdf(), Init(), LeapfrogStep(), Trajectory(), and VelocityVerletStep().

3.58.3.125 result

```
char result[250]  [extern]
```

Referenced by main().

3.58.3.126 rfAtom

```
double rfAtom  [extern]
```

Referenced by ComputeForcesCells(), and EvalVacf().

3.58.3.127 ro

```
double * ro
```

Definition at line 36 of file global.h.

Referenced by Close(), ComputeBondForce(), DumpBonds(), DumpRestart(), and Init().

3.58.3.128 rx

```
double* rx  [extern]
```

Referenced by ApplyBoundaryCond(), ApplyLeesEdwardsBoundaryCond(), ApplyShear(), BrownianStep(), Close(), ComputeBondForce(), ComputeForcesCells(), ComputePairForce(), DisplaceAtoms(), DumpRestart(), DumpState(), EvalRdf(), EvalSpacetimeCorr(), EvalUnwrap(), Init(), LeapfrogStep(), Trajectory(), and VelocityVerletStep().

3.58.3.129 rxUnwrap

```
double* rxUnwrap  [extern]
```

Referenced by Close(), EvalCom(), EvalUnwrap(), and Init().

3.58.3.130 ry

```
double * ry
```

Definition at line 17 of file global.h.

Referenced by ApplyBoundaryCond(), ApplyLeesEdwardsBoundaryCond(), ApplyShear(), BrownianStep(), Close(), ComputeBondForce(), ComputeForcesCells(), ComputePairForce(), DisplaceAtoms(), DumpRestart(), DumpState(), EvalRdf(), EvalUnwrap(), Init(), LeapfrogStep(), Trajectory(), and VelocityVerletStep().

3.58.3.131 ryUnwrap

```
double * ryUnwrap
```

Definition at line 48 of file global.h.

Referenced by Close(), EvalCom(), EvalUnwrap(), and Init().

3.58.3.132 shearDisplacement

```
double shearDisplacement  [extern]
```

Referenced by ApplyLeesEdwardsBoundaryCond(), ComputeBondForce(), ComputePairForce(), and Init().

3.58.3.133 shearVelocity

```
double shearVelocity
```

Definition at line 42 of file global.h.

Referenced by Init().

3.58.3.134 size

```
int size
```

Definition at line 79 of file global.h.

Referenced by ComputeForcesCells().

3.58.3.135 sizeHistRdf

```
int sizeHistRdf
```

Definition at line 99 of file global.h.

Referenced by AllocArrays(), EvalRdf(), and Init().

3.58.3.136 sKinEnergy

```
double sKinEnergy
```

Definition at line 21 of file global.h.

Referenced by AccumProps().

3.58.3.137 solver

```
char solver[128]  [extern]
```

Referenced by EvalProps(), and Init().

3.58.3.138 spacetimeCorr

```
double ** spacetimeCorr
```

Definition at line 89 of file global.h.

Referenced by AllocArrays(), Close(), and EvalSpacetimeCorr().

3.58.3.139 spacetimeCorrAv

```
double * spacetimeCorrAv
```

Definition at line 89 of file global.h.

Referenced by AllocArrays(), Close(), EvalSpacetimeCorr(), and SetupJob().

3.58.3.140 speed

```
double* speed  [extern]
```

Referenced by Close(), and Init().

3.58.3.141 sPotEnergy

```
double sPotEnergy
```

Definition at line 21 of file global.h.

Referenced by AccumProps().

3.58.3.142 sPressure

```
double sPressure
```

Definition at line 22 of file global.h.

Referenced by AccumProps().

3.58.3.143 SqrRadiusIJ

```
double SqrRadiusIJ
```

Definition at line 26 of file global.h.

Referenced by ComputeForcesCells(), and ComputePairForce().

3.58.3.144 ssKinEnergy

```
double ssKinEnergy
```

Definition at line 22 of file global.h.

Referenced by AccumProps().

3.58.3.145 ssPotEnergy

```
double ssPotEnergy
```

Definition at line 22 of file global.h.

Referenced by AccumProps().

3.58.3.146 ssPressure

```
double ssPressure
```

Definition at line 22 of file global.h.

Referenced by AccumProps().

3.58.3.147 ssTotEnergy

```
double ssTotEnergy
```

Definition at line 22 of file global.h.

Referenced by AccumProps().

3.58.3.148 stepAcf

```
int stepAcf
```

Definition at line 95 of file global.h.

Referenced by AccumVacf(), Init(), and PrintVacf().

3.58.3.149 stepAvg

```
int stepAvg
```

Definition at line 24 of file global.h.

Referenced by AccumProps(), Init(), and main().

3.58.3.150 stepCorr

```
int stepCorr
```

Definition at line 90 of file global.h.

Referenced by EvalSpacetimeCorr(), and Init().

3.58.3.151 stepCount

```
int stepCount
```

Definition at line 24 of file global.h.

Referenced by BrownianStep(), ComputeBondForce(), ComputePairForce(), HaltConditionCheck(), LeapfrogStep(), main(), and SetupJob().

3.58.3.152 stepDump

```
int stepDump
```

Definition at line 24 of file global.h.

Referenced by Init(), and main().

3.58.3.153 stepEquil

```
int stepEquil
```

Definition at line 24 of file global.h.

Referenced by BrownianStep(), Init(), and LeapfrogStep().

3.58.3.154 stepLimit

```
int stepLimit
```

Definition at line 24 of file global.h.

Referenced by Init(), and main().

3.58.3.155 stepRdf

```
int stepRdf
```

Definition at line 99 of file global.h.

Referenced by Init().

3.58.3.156 stepTraj

```
int stepTraj
```

Definition at line 24 of file global.h.

Referenced by Init(), and main().

3.58.3.157 sTotEnergy

```
double sTotEnergy
```

Definition at line 22 of file global.h.

Referenced by AccumProps().

3.58.3.158 strain

```
double strain  [extern]
```

Referenced by ApplyShear(), and Init().

3.58.3.159 strainRate

```
double strainRate
```

Definition at line 41 of file global.h.

Referenced by Init().

3.58.3.160 strech

```
double strech  [extern]
```

Referenced by ComputeBondForce(), and ComputePairForce().

3.58.3.161 stress

```
char stress[256]  [extern]
```

3.58.3.162 svirSum

```
double svirSum
```

Definition at line 21 of file global.h.

Referenced by AccumProps().

3.58.3.163 thermo

```
char thermo  [extern]
```

Referenced by Init(), and LeapfrogStep().

3.58.3.164 timeNow

```
double timeNow
```

Definition at line 20 of file global.h.

Referenced by DumpBonds(), DumpPairs(), DumpRestart(), DumpState(), EvalCom(), EvalRdf(), Init(), main(), PrintCom(), PrintMomentum(), PrintStress(), PrintSummary(), PrintVrms(), and Trajectory().

3.58.3.165 TotalBondEnergy

```
double TotalBondEnergy  [extern]
```

Referenced by ComputeBondForce(), and EvalProps().

3.58.3.166 TotalMass

```
double TotalMass
```

Definition at line 31 of file global.h.

Referenced by EvalCom().

3.58.3.167 totEnergy

```
double totEnergy
```

Definition at line 20 of file global.h.

Referenced by AccumProps(), EvalProps(), and PrintSummary().

3.58.3.168 uSum

```
double uSum
```

Definition at line 21 of file global.h.

Referenced by ComputeForcesCells().

3.58.3.169 uSumPair

```
double uSumPair  [extern]
```

Referenced by ComputePairForce(), and EvalProps().

3.58.3.170 uSumPairPerAtom

```
double uSumPairPerAtom
```

Definition at line 83 of file global.h.

Referenced by EvalProps(), and PrintSummary().

3.58.3.171 virSum

```
double virSum
```

Definition at line 21 of file global.h.

Referenced by AccumProps(), ComputeForcesCells(), EvalProps(), and PrintSummary().

3.58.3.172 virSumBond

```
double virSumBond  [extern]
```

Referenced by ComputeBondForce(), and EvalProps().

3.58.3.173 virSumBondxx

```
double virSumBondxx
```

Definition at line 84 of file global.h.

Referenced by ComputeBondForce(), and EvalProps().

3.58.3.174 virSumBondxy

```
double virSumBondxy
```

Definition at line 84 of file global.h.

Referenced by ComputeBondForce(), and EvalProps().

3.58.3.175 virSumBondyy

```
double virSumBondyy
```

Definition at line 84 of file global.h.

Referenced by ComputeBondForce(), and EvalProps().

3.58.3.176 virSumPair

```
double virSumPair
```

Definition at line 83 of file global.h.

Referenced by ComputePairForce(), and EvalProps().

3.58.3.177 virSumPairxx

```
double virSumPairxx
```

Definition at line 83 of file global.h.

Referenced by ComputePairForce(), and EvalProps().

3.58.3.178 virSumPairxy

```
double virSumPairxy
```

Definition at line 83 of file global.h.

Referenced by ComputePairForce(), and EvalProps().

3.58.3.179 virSumPairyy

```
double virSumPairyy
```

Definition at line 83 of file global.h.

Referenced by ComputePairForce(), and EvalProps().

3.58.3.180 virSumxx

```
double virSumxx  [extern]
```

Referenced by EvalProps(), and PrintStress().

3.58.3.181 virSumxy

```
double virSumxy
```

Definition at line 85 of file global.h.

Referenced by EvalProps(), and PrintStress().

3.58.3.182 virSumyy

```
double virSumyy
```

Definition at line 85 of file global.h.

Referenced by EvalProps(), and PrintStress().

3.58.3.183 visc

```
char visc[256]  [extern]
```

3.58.3.184 viscAcf

```
double ** viscAcf
```

Definition at line 94 of file global.h.

Referenced by AccumVacf(), AllocArrays(), Close(), and EvalVacf().

3.58.3.185 viscAcfAv

```
double * viscAcfAv
```

Definition at line 94 of file global.h.

Referenced by AccumVacf(), AllocArrays(), Close(), PrintVacf(), and ZeroVacf().

3.58.3.186 viscAcfInt

```
double viscAcfInt
```

Definition at line 94 of file global.h.

Referenced by AccumVacf(), and PrintVacf().

3.58.3.187 viscAcfOrg

```
double * viscAcfOrg
```

Definition at line 94 of file global.h.

Referenced by AllocArrays(), Close(), and EvalVacf().

3.58.3.188 VMeanSqr

```
double VMeanSqr
```

Definition at line 43 of file global.h.

Referenced by EvalVrms().

3.58.3.189 vrms

```
char vrms[256]  [extern]
```

Referenced by main().

3.58.3.190 VRootMeanSqr

```
double VRootMeanSqr
```

Definition at line 43 of file global.h.

Referenced by EvalVrms(), main(), and PrintVrms().

3.58.3.191 VSqr

```
double VSqr  [extern]
```

Referenced by EvalVrms().

3.58.3.192 vSum

```
double vSum
```

Definition at line 21 of file global.h.

Referenced by EvalProps(), and PrintSummary().

3.58.3.193 vSumX

```
double vSumX
```

Definition at line 21 of file global.h.

Referenced by EvalProps(), and PrintMomentum().

3.58.3.194 vSumY

```
double vSumY
```

Definition at line 21 of file global.h.

Referenced by EvalProps(), and PrintMomentum().

3.58.3.195 vvSum

```
double vvSum
```

Definition at line 21 of file global.h.

Referenced by EvalProps(), and LeapfrogStep().

3.58.3.196 vx

```
double * vx
```

Definition at line 17 of file global.h.

Referenced by ApplyBoundaryCond(), ApplyDrivingForce(), ApplyViscous(), BrownianStep(), Close(), ComputeBondForce(), ComputeForcesCells(), ComputePairForce(), DumpRestart(), DumpState(), EvalProps(), EvalVacf(), EvalVrms(), Init(), LeapfrogStep(), Trajectory(), and VelocityVerletStep().

3.58.3.197 vy

```
double * vy
```

Definition at line 17 of file global.h.

Referenced by ApplyBoundaryCond(), ApplyDrivingForce(), ApplyViscous(), BrownianStep(), Close(), ComputeBondForce(), ComputeForcesCells(), ComputePairForce(), DumpRestart(), DumpState(), EvalProps(), EvalVacf(), EvalVrms(), Init(), LeapfrogStep(), Trajectory(), and VelocityVerletStep().

3.58.3.198 xBoundary

```
char xBoundary[10]  [extern]
```

Referenced by ApplyBoundaryCond(), and Init().

3.58.3.199 xyz

```
char xyz[256]  [extern]
```

Referenced by main().

3.58.3.200 yBoundary

```
char yBoundary[10]
```

Definition at line 64 of file global.h.

Referenced by ApplyBoundaryCond(), and Init().

3.59 global.h

Go to the documentation of this file.

```
00001 #ifndef GLOBAL_H
00002 #define GLOBAL_H
00003 #include <stdio.h>  // Required for FILE*
00004
00005 #ifdef DEFINE_GLOBALS
00006     #define EXTERN
00007 #else
00008     #define EXTERN extern
00009 #endif
00010
00011 typedef double real;
00012
00013 #define NDIM 2
00014 #define Sqr(x) ((x) * (x))
00015 #define SignR(x, y) (((y) >= 0) ? (x) : (- (x)))
00016
00017 EXTERN double *rx, *ry, *vx, *vy, *ax, *ay;
00018 EXTERN double *speed;
00019
00020 EXTERN double region[NDIM+1], regionH[NDIM+1], deltaT, timeNow, potEnergy, kinEnergy, totEnergy,
00021 density, pressure, rCut, kappa, uSum, virSum, svirSum, vSum, vSumX, vSumY, vvSum, sPotEnergy,
      sKinEnergy,
00022 sTotEnergy, sPressure, ssPotEnergy, ssKinEnergy, ssTotEnergy, ssPressure;
00023
00024 EXTERN int     initUcell[NDIM+1], moreCycles, nAtom, stepAvg, stepCount, stepEquil, stepLimit,
      stepTraj, stepDump;
00025
00026 EXTERN double  RadiusIJ, SqrRadiusIJ, RadiusIJInv;
00027 EXTERN int     nAtomType;
00028 EXTERN int     *atomType;
00029 EXTERN int     *atomID;
00030 EXTERN double  *atomRadius;
00031 EXTERN double  *atomMass, TotalMass;
00032
00033 EXTERN int     nBond, nBondType;
00034 EXTERN int     *atom1, *atom2;
00035 EXTERN int     *BondID, *BondType ;
00036 EXTERN double  *kb, *ro;
00037 EXTERN double  *BondEnergy, *BondLength;
00038 EXTERN double  TotalBondEnergy, BondEnergyPerAtom;
00039 EXTERN double  gamman;
00040 EXTERN double  *discDragx, *discDragy, *nodeDragx, *nodeDragy;
00041 EXTERN double  strain, strainRate;
00042 EXTERN double  shearDisplacement, shearVelocity;
00043 EXTERN double  VSqr, VMeanSqr, VRootMeanSqr;
00044 EXTERN double  ComX, ComY, ComX0, ComY0, ComXRatio, ComYRatio;
00045 EXTERN double  HaltCondition;
00046 EXTERN double  DeltaY, DeltaX;
00047 EXTERN int     *ImageX, *ImageY;
00048 EXTERN double  *rxUnwrap, *ryUnwrap;
00049 EXTERN int     nAtomInterface, nDiscInterface,  nAtomBlock;
00050 EXTERN int     *atomIDInterface;
00051 EXTERN double  Kn;
00052 EXTERN double  fx, fy, FyBylx, fxByfy;
00053 EXTERN int     DampFlag;
```

```
00054 EXTERN double  strech;
00055
00056 //For dumping the pair interaction data
00057 EXTERN int     dumpPairFlag;
00058 EXTERN int     nPairTotal, nPairActive;
00059 EXTERN int     *PairID, *Pairatom1, *Pairatom2;
00060 EXTERN double  *PairXij, *PairYij;
00061
00062
00063 EXTERN char   solver[128];
00064 EXTERN char   xBoundary[10], yBoundary[10];
00065 EXTERN char    thermo;
00066
00067 //For damping as in PRL, 130, 178203 (2023)
00068 EXTERN double *DeltaXijOld, *DeltaYijOld;
00069 EXTERN double DeltaXijNew, DeltaYijNew;
00070 EXTERN double DeltaXij, DeltaYij, DeltaVXij, DeltaVYij;
00071 EXTERN double **DeltaXijOldPair, **DeltaYijOldPair;
00072
00073 //For molecule-ID as per LAMMPS, helpful!
00074 EXTERN int    *molID;
00075 EXTERN int    **isBonded;
00076
00077 //Following three for MPI only
00078 EXTERN int     *cellList, cells[NDIM+1];
00079 EXTERN int     rank, size, master;
00080 EXTERN double  *fax, *fay, fuSum, fvirSum, frfAtom;
00081
00082 //For thermodynamic properties
00083 EXTERN double  uSumPair, uSumPairPerAtom, virSumPair, virSumPairxx, virSumPairyy, virSumPairxy;
00084 EXTERN double  virSumBond, virSumBondxx, virSumBondyy, virSumBondxy;
00085 EXTERN double  virSumxx, virSumyy, virSumxy;
00086 EXTERN int     freezeAtomType;
00087
00088 // Spacetime Correlations
00089 EXTERN double  **cfOrg, **spacetimeCorr, *cfVal, *spacetimeCorrAv;
00090 EXTERN int     *indexCorr, countCorrAv, limitCorrAv, nBuffCorr, nFunCorr, nValCorr, stepCorr;
00091
00092 // Viscosity
00093 EXTERN double  rfAtom, frfAtom;
00094 EXTERN double  *indexAcf, **viscAcf, *viscAcfOrg, *viscAcfAv, viscAcfInt;
00095 EXTERN int      nValAcf, nBuffAcf, stepAcf, countAcfAv, limitAcfAv;
00096
00097 // Radial distribution function
00098 EXTERN double  *histRdf, rangeRdf;
00099 EXTERN int     countRdf, limitRdf, sizeHistRdf, stepRdf;
00100
00101
00102 // Output files prefixes
00103 EXTERN char      *prefix;
00104
00105 EXTERN char    result[250];
00106 EXTERN FILE    *fpresult;
00107
00108 EXTERN char    xyz[256];
00109 EXTERN FILE    *fpxyz;
00110
00111 EXTERN char    bond[256];
00112 EXTERN FILE    *fpbond;
00113
00114
00115 EXTERN char    dump[256];
00116 EXTERN FILE    *fpdump;
00117
00118 EXTERN char    dnsty[256];
00119 EXTERN FILE    *fpdnsty;
00120
00121 EXTERN char    visc[256];
00122 EXTERN FILE    *fpvisc;
00123
00124 EXTERN char    rdf[256];
00125 EXTERN FILE    *fprdf;
00126
00127 EXTERN char    vrms[256];
00128 EXTERN FILE    *fpvrms;
00129
00130 EXTERN char    stress[256];
00131 EXTERN FILE    *fpstress;
00132
00133 EXTERN char    momentum[256];
00134 EXTERN FILE    *fpmomentum;
00135
00136 EXTERN char    com[256];
00137 EXTERN FILE    *fpcom;
00138
00139 EXTERN char    pair[256];
00140 EXTERN FILE    *fppair;
```

```
00141
00142 #endif // GLOBALEXTERN_H
```

3.60 source/globalExtern.h File Reference

Macros

- #define NDIM 2
- #define Sqr(x) ((x) ∗ (x))
- #define SignR(x, y) (((y) >= 0) ? (x) : (- (x)))

Typedefs

- typedef double real

Variables

- double ∗ rx
- double ∗ ry
- double ∗ vx
- double ∗ vy
- double ∗ ax
- double ∗ ay
- double ∗ speed
- double region [2+1]
- double regionH [2+1]
- double deltaT
- double timeNow
- double potEnergy
- double kinEnergy
- double totEnergy
- double density
- double pressure
- double rCut
- double kappa
- double uSum
- double virSum
- double svirSum
- double vSum
- double vSumX
- double vSumY
- double vvSum
- double sPotEnergy
- double sKinEnergy
- double sTotEnergy
- double sPressure
- double ssPotEnergy
- double ssKinEnergy
- double ssTotEnergy
- double ssPressure
- int initUcell [2+1]

- int moreCycles
- int nAtom
- int stepAvg
- int stepCount
- int stepEquil
- int stepLimit
- int stepTraj
- int stepDump
- double RadiusIJ
- double SqrRadiusIJ
- double RadiusIJInv
- int nAtomType
- int * atomType
- int * atomID
- double * atomRadius
- double * atomMass
- double TotalMass
- int nBond
- int nBondType
- int * atom1
- int * atom2
- int * BondID
- int * BondType
- double * kb
- double * ro
- double * BondEnergy
- double * BondLength
- double TotalBondEnergy
- double BondEnergyPerAtom
- double gamman
- double * discDragx
- double * discDragy
- double * nodeDragx
- double * nodeDragy
- double strain
- double strainRate
- double shearDisplacement
- double shearVelocity
- double VSqr
- double VMeanSqr
- double VRootMeanSqr
- double ComX
- double ComY
- double ComX0
- double ComY0
- double ComXRatio
- double ComYRatio
- double HaltCondition
- double DeltaY
- double DeltaX
- int * ImageX
- int * ImageY
- double * rxUnwrap
- double * ryUnwrap
- int nAtomInterface

- int nDiscInterface
- int nAtomBlock
- int * atomIDInterface
- double Kn
- double fx
- double fy
- double FyBylx
- double fxByfy
- int DampFlag
- double strech
- int dumpPairFlag
- int nPairTotal
- int nPairActive
- int * PairID
- int * Pairatom1
- int * Pairatom2
- double * PairXij
- double * PairYij
- char solver [128]
- char xBoundary [10]
- char yBoundary [10]
- double * DeltaXijOld
- double * DeltaYijOld
- double DeltaXijNew
- double DeltaYijNew
- double DeltaXij
- double DeltaYij
- double DeltaVXij
- double DeltaVYij
- double ** DeltaXijOldPair
- double ** DeltaYijOldPair
- int * molID
- int ** isBonded
- int * cellList
- int cells [2+1]
- int rank
- int size
- int master
- double * fax
- double * fay
- double fuSum
- double fvirSum
- double frfAtom
- double uSumPair
- double uSumPairPerAtom
- double virSumPair
- double virSumPairxx
- double virSumPairyy
- double virSumPairxy
- double virSumBond
- double virSumBondxx
- double virSumBondyy
- double virSumBondxy
- double virSumxx
- double virSumyy

- double virSumxy
- int freezeAtomType
- double ** cfOrg
- double ** spacetimeCorr
- double * cfVal
- double * spacetimeCorrAv
- int * indexCorr
- int countCorrAv
- int limitCorrAv
- int nBuffCorr
- int nFunCorr
- int nValCorr
- int stepCorr
- double rfAtom
- double * indexAcf
- double ** viscAcf
- double * viscAcfOrg
- double * viscAcfAv
- double viscAcfInt
- int nValAcf
- int nBuffAcf
- int stepAcf
- int countAcfAv
- int limitAcfAv
- double * histRdf
- double rangeRdf
- int countRdf
- int limitRdf
- int sizeHistRdf
- int stepRdf
- char * prefix
- char result [250]
- FILE * fpresult
- char xyz [256]
- FILE * fpxyz
- char bond [256]
- FILE * fpbond
- char dump [256]
- FILE * fpdump
- char dnsty [256]
- FILE * fpdnsty
- char visc [256]
- FILE * fpvisc
- char rdf [256]
- FILE * fprdf
- char vrms [256]
- FILE * fpvrms
- char stress [256]
- FILE * fpstress
- char momentum [256]
- FILE * fpmomentum
- char com [256]
- FILE * fpcom
- char pair [256]
- FILE * fppair

3.60.1 Macro Definition Documentation

3.60.1.1 NDIM

```
#define NDIM 2
```

Definition at line 6 of file globalExtern.h.

3.60.1.2 SignR

```
#define SignR(
              x,
              y ) (((y) >= 0) ?  (x) :  (- (x)))
```

Definition at line 8 of file globalExtern.h.

3.60.1.3 Sqr

```
#define Sqr(
              x ) ((x) * (x))
```

Definition at line 7 of file globalExtern.h.

3.60.2 Typedef Documentation

3.60.2.1 real

```
typedef double real
```

Definition at line 4 of file globalExtern.h.

3.60.3 Variable Documentation

3.60.3.1 atom1

```
int* atom1  [extern]
```

3.60.3.2 atom2

```
int * atom2
```

Definition at line 27 of file globalExtern.h.

3.60.3.3 atomID

```
int* atomID  [extern]
```

3.60.3.4 atomIDInterface

```
int* atomIDInterface  [extern]
```

3.60.3.5 atomMass

```
double* atomMass  [extern]
```

3.60.3.6 atomRadius

```
double* atomRadius  [extern]
```

3.60.3.7 atomType

```
int* atomType  [extern]
```

3.60.3.8 ax

```
double * ax
```

Definition at line 10 of file globalExtern.h.

3.60.3.9 ay

```
double * ay
```

Definition at line 10 of file globalExtern.h.

3.60.3.10 bond

```
char bond[256]  [extern]
```

3.60.3.11 BondEnergy

```
double* BondEnergy  [extern]
```

3.60.3.12 BondEnergyPerAtom

```
double BondEnergyPerAtom
```

Definition at line 31 of file globalExtern.h.

3.60.3.13 BondID

```
int* BondID  [extern]
```

3.60.3.14 BondLength

```
double * BondLength
```

Definition at line 30 of file globalExtern.h.

3.60.3.15 BondType

```
int * BondType
```

Definition at line 28 of file globalExtern.h.

3.60.3.16 cellList

```
int* cellList  [extern]
```

3.60.3.17 cells

```
int cells[2+1]
```

Definition at line 70 of file globalExtern.h.

3.60.3.18 cfOrg

```
double** cfOrg  [extern]
```

3.60.3.19 cfVal

```
double * cfVal
```

Definition at line 81 of file globalExtern.h.

3.60.3.20 com

```
char com[256]  [extern]
```

3.60.3.21 ComX

```
double ComX  [extern]
```

3.60.3.22 ComX0

```
double ComX0
```

Definition at line 37 of file globalExtern.h.

3.60.3.23 ComXRatio

```
double ComXRatio
```

Definition at line 37 of file globalExtern.h.

3.60.3.24 ComY

```
double ComY
```

Definition at line 37 of file globalExtern.h.

3.60.3.25 ComY0

```
double ComY0
```

Definition at line 37 of file globalExtern.h.

3.60.3.26 ComYRatio

```
double ComYRatio
```

Definition at line 37 of file globalExtern.h.

3.60.3.27 countAcfAv

```
int countAcfAv
```

Definition at line 87 of file globalExtern.h.

3.60.3.28 countCorrAv

```
int countCorrAv
```

Definition at line 82 of file globalExtern.h.

3.60.3.29 countRdf

```
int countRdf  [extern]
```

3.60.3.30 DampFlag

```
int DampFlag  [extern]
```

3.60.3.31 deltaT

```
double deltaT
```

Definition at line 13 of file globalExtern.h.

3.60.3.32 DeltaVXij

```
double DeltaVXij
```

Definition at line 62 of file globalExtern.h.

3.60.3.33 DeltaVYij

```
double DeltaVYij
```

Definition at line 62 of file globalExtern.h.

3.60.3.34 DeltaX

```
double DeltaX
```

Definition at line 39 of file globalExtern.h.

3.60.3.35 DeltaXij

```
double DeltaXij  [extern]
```

3.60.3.36 DeltaXijNew

```
double DeltaXijNew  [extern]
```

3.60.3.37 DeltaXijOld

```
double* DeltaXijOld  [extern]
```

3.60.3.38 DeltaXijOldPair

```
double** DeltaXijOldPair  [extern]
```

3.60.3.39 DeltaY

```
double DeltaY  [extern]
```

3.60.3.40 DeltaYij

```
double DeltaYij
```

Definition at line 62 of file globalExtern.h.

3.60.3.41 DeltaYijNew

```
double DeltaYijNew
```

Definition at line 61 of file globalExtern.h.

3.60.3.42 DeltaYijOld

```
double * DeltaYijOld
```

Definition at line 60 of file globalExtern.h.

3.60.3.43 DeltaYijOldPair

```
double ** DeltaYijOldPair
```

Definition at line 63 of file globalExtern.h.

3.60.3.44 density

```
double density
```

Definition at line 14 of file globalExtern.h.

3.60.3.45 discDragx

```
double* discDragx  [extern]
```

3.60.3.46 discDragy

```
double * discDragy
```

Definition at line 33 of file globalExtern.h.

3.60.3.47 dnsty

```
char dnsty[256]  [extern]
```

3.60.3.48 dump

```
char dump[256]  [extern]
```

3.60.3.49 dumpPairFlag

```
int dumpPairFlag  [extern]
```

3.60.3.50 fax

```
double* fax  [extern]
```

3.60.3.51 fay

```
double * fay
```

Definition at line 72 of file globalExtern.h.

3.60.3.52 fpbond

```
FILE* fpbond  [extern]
```

3.60.3.53 fpcom

```
FILE* fpcom  [extern]
```

3.60.3.54 fpdnsty

```
FILE* fpdnsty  [extern]
```

3.60.3.55 fpdump

```
FILE* fpdump  [extern]
```

3.60.3.56 fpmomentum

```
FILE* fpmomentum  [extern]
```

3.60.3.57 fppair

```
FILE* fppair  [extern]
```

3.60.3.58 fprdf

```
FILE* fprdf  [extern]
```

3.60.3.59 fpresult

```
FILE* fpresult  [extern]
```

3.60.3.60 fpstress

```
FILE* fpstress  [extern]
```

3.60.3.61 fpvisc

```
FILE* fpvisc  [extern]
```

3.60.3.62 fpvrms

```
FILE* fpvrms  [extern]
```

3.60.3.63 fpxyz

```
FILE* fpxyz  [extern]
```

3.60.3.64 freezeAtomType

```
int freezeAtomType  [extern]
```

3.60.3.65 frfAtom

```
double frfAtom
```

Definition at line 72 of file globalExtern.h.

3.60.3.66 fuSum

```
double fuSum
```

Definition at line 72 of file globalExtern.h.

3.60.3.67 fvirSum

```
double fvirSum
```

Definition at line 72 of file globalExtern.h.

3.60.3.68 fx

```
double fx  [extern]
```

3.60.3.69 fxByfy

```
double fxByfy
```

Definition at line 45 of file globalExtern.h.

3.60.3.70 fy

```
double fy
```

Definition at line 45 of file globalExtern.h.

3.60.3.71 FyBylx

```
double FyBylx
```

Definition at line 45 of file globalExtern.h.

3.60.3.72 gamman

```
double gamman  [extern]
```

3.60.3.73 HaltCondition

```
double HaltCondition  [extern]
```

3.60.3.74 histRdf

```
double* histRdf  [extern]
```

3.60.3.75 ImageX

```
int* ImageX  [extern]
```

3.60.3.76 ImageY

```
int * ImageY
```

Definition at line 40 of file globalExtern.h.

3.60.3.77 indexAcf

```
double* indexAcf  [extern]
```

3.60.3.78 indexCorr

```
int* indexCorr  [extern]
```

3.60.3.79 initUcell

```
int initUcell[2+1]  [extern]
```

3.60.3.80 isBonded

```
int** isBonded  [extern]
```

3.60.3.81 kappa

```
double kappa
```

Definition at line 14 of file globalExtern.h.

3.60.3.82 kb

```
double* kb  [extern]
```

3.60.3.83 kinEnergy

```
double kinEnergy
```

Definition at line 13 of file globalExtern.h.

3.60.3.84 Kn

```
double Kn  [extern]
```

3.60.3.85 limitAcfAv

```
int limitAcfAv
```

Definition at line 87 of file globalExtern.h.

3.60.3.86 limitCorrAv

```
int limitCorrAv
```

Definition at line 82 of file globalExtern.h.

3.60.3.87 limitRdf

```
int limitRdf
```

Definition at line 91 of file globalExtern.h.

3.60.3.88 master

```
int master
```

Definition at line 71 of file globalExtern.h.

3.60.3.89 molID

```
int* molID  [extern]
```

3.60.3.90 momentum

```
char momentum[256]  [extern]
```

3.60.3.91 moreCycles

```
int moreCycles
```

Definition at line 17 of file globalExtern.h.

3.60.3.92 nAtom

```
int nAtom
```

Definition at line 17 of file globalExtern.h.

3.60.3.93 nAtomBlock

```
int nAtomBlock
```

Definition at line 42 of file globalExtern.h.

3.60.3.94 nAtomInterface

```
int nAtomInterface  [extern]
```

3.60.3.95 nAtomType

```
int nAtomType  [extern]
```

3.60.3.96 nBond

```
int nBond  [extern]
```

3.60.3.97 nBondType

```
int nBondType
```

Definition at line 26 of file globalExtern.h.

3.60.3.98 nBuffAcf

```
int nBuffAcf
```

Definition at line 87 of file globalExtern.h.

3.60.3.99 nBuffCorr

```
int nBuffCorr
```

Definition at line 82 of file globalExtern.h.

3.60.3.100 nDiscInterface

```
int nDiscInterface
```

Definition at line 42 of file globalExtern.h.

3.60.3.101 nFunCorr

```
int nFunCorr
```

Definition at line 82 of file globalExtern.h.

3.60.3.102 nodeDragx

```
double * nodeDragx
```

Definition at line 33 of file globalExtern.h.

3.60.3.103 nodeDragy

```
double * nodeDragy
```

Definition at line 33 of file globalExtern.h.

3.60.3.104 nPairActive

```
int nPairActive
```

Definition at line 51 of file globalExtern.h.

3.60.3.105 nPairTotal

```
int nPairTotal  [extern]
```

3.60.3.106 nValAcf

```
int nValAcf  [extern]
```

3.60.3.107 nValCorr

```
int nValCorr
```

Definition at line 82 of file globalExtern.h.

3.60.3.108 pair

```
char pair[256]  [extern]
```

3.60.3.109 Pairatom1

```
int * Pairatom1
```

Definition at line 52 of file globalExtern.h.

3.60.3.110 Pairatom2

```
int * Pairatom2
```

Definition at line 52 of file globalExtern.h.

3.60.3.111 PairID

```
int* PairID  [extern]
```

3.60.3.112 PairXij

```
double* PairXij  [extern]
```

3.60.3.113 PairYij

```
double * PairYij
```

Definition at line 53 of file globalExtern.h.

3.60.3.114 potEnergy

```
double potEnergy
```

Definition at line 13 of file globalExtern.h.

3.60.3.115 prefix

```
char* prefix  [extern]
```

Definition at line 13 of file main.c.

Referenced by main().

3.60.3.116 pressure

```
double pressure
```

Definition at line 14 of file globalExtern.h.

3.60.3.117 RadiusIJ

```
double RadiusIJ  [extern]
```

3.60.3.118 RadiusIJInv

```
double RadiusIJInv
```

Definition at line 19 of file globalExtern.h.

3.60.3.119 rangeRdf

```
double rangeRdf
```

Definition at line 90 of file globalExtern.h.

3.60.3.120 rank

```
int rank  [extern]
```

3.60.3.121 rCut

```
double rCut
```

Definition at line 14 of file globalExtern.h.

3.60.3.122 rdf

```
char rdf[256]  [extern]
```

3.60.3.123 region

```
double region[2+1]  [extern]
```

3.60.3.124 regionH

```
double regionH[2+1]
```

Definition at line 13 of file globalExtern.h.

3.60.3.125 result

```
char result[250]  [extern]
```

3.60.3.126 rfAtom

```
double rfAtom  [extern]
```

3.60.3.127 ro

```
double * ro
```

Definition at line 29 of file globalExtern.h.

3.60.3.128 rx

```
double* rx  [extern]
```

3.60.3.129 rxUnwrap

```
double* rxUnwrap  [extern]
```

3.60.3.130 ry

```
double * ry
```

Definition at line 10 of file globalExtern.h.

3.60.3.131 ryUnwrap

```
double * ryUnwrap
```

Definition at line 41 of file globalExtern.h.

3.60.3.132 shearDisplacement

```
double shearDisplacement  [extern]
```

3.60.3.133 shearVelocity

```
double shearVelocity
```

Definition at line 35 of file globalExtern.h.

3.60.3.134 size

```
int size
```

Definition at line 71 of file globalExtern.h.

3.60.3.135 sizeHistRdf

```
int sizeHistRdf
```

Definition at line 91 of file globalExtern.h.

3.60.3.136 sKinEnergy

```
double sKinEnergy
```

Definition at line 14 of file globalExtern.h.

3.60.3.137 solver

```
char solver[128]  [extern]
```

3.60.3.138 spacetimeCorr

```
double ** spacetimeCorr
```

Definition at line 81 of file globalExtern.h.

3.60.3.139 spacetimeCorrAv

```
double * spacetimeCorrAv
```

Definition at line 81 of file globalExtern.h.

3.60.3.140 speed

```
double* speed  [extern]
```

3.60.3.141 sPotEnergy

```
double sPotEnergy
```

Definition at line 14 of file globalExtern.h.

3.60.3.142 sPressure

```
double sPressure
```

Definition at line 15 of file globalExtern.h.

3.60.3.143 SqrRadiusIJ

```
double SqrRadiusIJ
```

Definition at line 19 of file globalExtern.h.

3.60.3.144 ssKinEnergy

```
double ssKinEnergy
```

Definition at line 15 of file globalExtern.h.

3.60.3.145 ssPotEnergy

```
double ssPotEnergy
```

Definition at line 15 of file globalExtern.h.

3.60.3.146 ssPressure

```
double ssPressure
```

Definition at line 15 of file globalExtern.h.

3.60.3.147 ssTotEnergy

```
double ssTotEnergy
```

Definition at line 15 of file globalExtern.h.

3.60.3.148 stepAcf

```
int stepAcf
```

Definition at line 87 of file globalExtern.h.

3.60.3.149 stepAvg

```
int stepAvg
```

Definition at line 17 of file globalExtern.h.

3.60.3.150 stepCorr

```
int stepCorr
```

Definition at line 82 of file globalExtern.h.

3.60.3.151 stepCount

```
int stepCount
```

Definition at line 17 of file globalExtern.h.

3.60.3.152 stepDump

```
int stepDump
```

Definition at line 17 of file globalExtern.h.

3.60.3.153 stepEquil

```
int stepEquil
```

Definition at line 17 of file globalExtern.h.

3.60.3.154 stepLimit

```
int stepLimit
```

Definition at line 17 of file globalExtern.h.

3.60.3.155 stepRdf

```
int stepRdf
```

Definition at line 91 of file globalExtern.h.

3.60.3.156 stepTraj

```
int stepTraj
```

Definition at line 17 of file globalExtern.h.

3.60.3.157 sTotEnergy

```
double sTotEnergy
```

Definition at line 15 of file globalExtern.h.

3.60.3.158 strain

```
double strain  [extern]
```

3.60.3.159 strainRate

```
double strainRate
```

Definition at line 34 of file globalExtern.h.

3.60.3.160 strech

```
double strech  [extern]
```

3.60.3.161 stress

```
char stress[256]  [extern]
```

3.60.3.162 svirSum

```
double svirSum
```

Definition at line 14 of file globalExtern.h.

3.60.3.163 timeNow

```
double timeNow
```

Definition at line 13 of file globalExtern.h.

3.60.3.164 TotalBondEnergy

```
double TotalBondEnergy  [extern]
```

3.60.3.165 TotalMass

```
double TotalMass
```

Definition at line 24 of file globalExtern.h.

3.60.3.166 totEnergy

```
double totEnergy
```

Definition at line 13 of file globalExtern.h.

3.60.3.167 uSum

```
double uSum
```

Definition at line 14 of file globalExtern.h.

3.60.3.168 uSumPair

```
double uSumPair  [extern]
```

3.60.3.169 uSumPairPerAtom

```
double uSumPairPerAtom
```

Definition at line 75 of file globalExtern.h.

3.60.3.170 virSum

```
double virSum
```

Definition at line 14 of file globalExtern.h.

3.60.3.171 virSumBond

```
double virSumBond  [extern]
```

3.60.3.172 virSumBondxx

```
double virSumBondxx
```

Definition at line 76 of file globalExtern.h.

3.60.3.173 virSumBondxy

```
double virSumBondxy
```

Definition at line 76 of file globalExtern.h.

3.60.3.174 virSumBondyy

```
double virSumBondyy
```

Definition at line 76 of file globalExtern.h.

3.60.3.175 virSumPair

```
double virSumPair
```

Definition at line 75 of file globalExtern.h.

3.60.3.176 virSumPairxx

```
double virSumPairxx
```

Definition at line 75 of file globalExtern.h.

3.60.3.177 virSumPairxy

```
double virSumPairxy
```

Definition at line 75 of file globalExtern.h.

3.60.3.178 virSumPairyy

```
double virSumPairyy
```

Definition at line 75 of file globalExtern.h.

3.60.3.179 virSumxx

```
double virSumxx  [extern]
```

3.60.3.180 virSumxy

```
double virSumxy
```

Definition at line 77 of file globalExtern.h.

3.60.3.181 virSumyy

```
double virSumyy
```

Definition at line 77 of file globalExtern.h.

3.60.3.182 visc

```
char visc[256]  [extern]
```

3.60.3.183 viscAcf

```
double ** viscAcf
```

Definition at line 86 of file globalExtern.h.

3.60.3.184 viscAcfAv

```
double * viscAcfAv
```

Definition at line 86 of file globalExtern.h.

3.60.3.185 viscAcfInt

```
double viscAcfInt
```

Definition at line 86 of file globalExtern.h.

3.60.3.186 viscAcfOrg

```
double * viscAcfOrg
```

Definition at line 86 of file globalExtern.h.

3.60.3.187 VMeanSqr

```
double VMeanSqr
```

Definition at line 36 of file globalExtern.h.

3.60.3.188 vrms

```
char vrms[256]  [extern]
```

3.60.3.189 VRootMeanSqr

```
double VRootMeanSqr
```

Definition at line 36 of file globalExtern.h.

3.60.3.190 VSqr

```
double VSqr  [extern]
```

3.60.3.191 vSum

```
double vSum
```

Definition at line 14 of file globalExtern.h.

3.60.3.192 vSumX

```
double vSumX
```

Definition at line 14 of file globalExtern.h.

3.60.3.193 vSumY

```
double vSumY
```

Definition at line 14 of file globalExtern.h.

3.60.3.194 vvSum

```
double vvSum
```

Definition at line 14 of file globalExtern.h.

3.60.3.195 vx

```
double * vx
```

Definition at line 10 of file globalExtern.h.

3.60.3.196 vy

```
double * vy
```

Definition at line 10 of file globalExtern.h.

3.60.3.197 xBoundary

```
char xBoundary[10]  [extern]
```

3.60.3.198 xyz

```
char xyz[256]  [extern]
```

3.60.3.199 yBoundary

```
char yBoundary[10]
```

Definition at line 57 of file globalExtern.h.

3.61 globalExtern.h

Go to the documentation of this file.

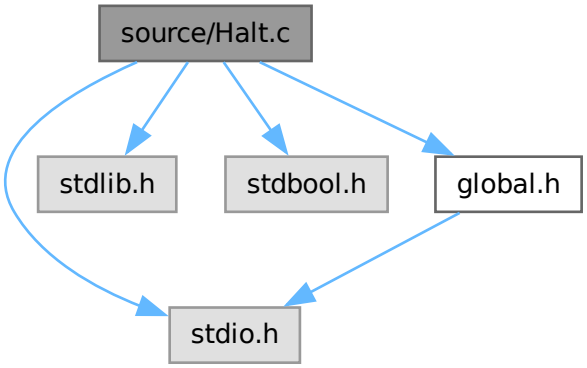
```
00001 #ifndef GLOBALEXTERN_H
00002 #define GLOBALEXTERN_H
00003
00004 typedef double real;
00005
00006 #define NDIM 2
00007 #define Sqr(x) ((x) * (x))
00008 #define SignR(x, y) (((y) >= 0) ? (x) : (- (x)))
00009
00010 extern double   *rx, *ry, *vx, *vy, *ax, *ay;
00011 extern double   *speed;
00012
00013 extern double   region[NDIM+1], regionH[NDIM+1], deltaT, timeNow, potEnergy, kinEnergy, totEnergy,
00014 density, pressure, rCut, kappa, uSum, virSum, svirSum, vSum, vSumX, vSumY, vvSum, sPotEnergy,
      sKinEnergy,
00015 sTotEnergy, sPressure, ssPotEnergy, ssKinEnergy, ssTotEnergy, ssPressure;
00016
00017 extern int     initUcell[NDIM+1], moreCycles, nAtom, stepAvg, stepCount, stepEquil, stepLimit,
      stepTraj, stepDump;
00018
00019 extern double  RadiusIJ, SqrRadiusIJ, RadiusIJInv;
00020 extern int     nAtomType;
00021 extern int     *atomType;
00022 extern int     *atomID;
00023 extern double  *atomRadius;
00024 extern double  *atomMass, TotalMass;
00025
00026 extern int     nBond, nBondType;
00027 extern int     *atom1, *atom2;
00028 extern int     *BondID, *BondType ;
00029 extern double  *kb, *ro;
00030 extern double  *BondEnergy, *BondLength;
00031 extern double  TotalBondEnergy, BondEnergyPerAtom;
00032 extern double  gamman;
00033 extern double  *discDragx, *discDragy, *nodeDragx, *nodeDragy;
00034 extern double  strain, strainRate;
00035 extern double  shearDisplacement, shearVelocity;
00036 extern double  VSqr, VMeanSqr, VRootMeanSqr;
00037 extern double  ComX, ComY, ComX0, ComY0, ComXRatio, ComYRatio;
00038 extern double  HaltCondition;
00039 extern double  DeltaY, DeltaX;
00040 extern int     *ImageX, *ImageY;
00041 extern double  *rxUnwrap, *ryUnwrap;
00042 extern int     nAtomInterface, nDiscInterface,  nAtomBlock;
00043 extern int     *atomIDInterface;
00044 extern double  Kn;
00045 extern double  fx, fy, FyBylx, fxByfy;
00046 extern int     DampFlag;
00047 extern double  strech;
00048
00049 //For dumping the pair interaction data
00050 extern int     dumpPairFlag;
00051 extern int     nPairTotal, nPairActive;
00052 extern int     *PairID, *Pairatom1, *Pairatom2;
00053 extern double  *PairXij, *PairYij;
00054
00055
00056 extern char solver[128];
00057 extern char xBoundary[10], yBoundary[10];
00058
00059 //For damping as in PRL, 130, 178203 (2023)
00060 extern double *DeltaXijOld, *DeltaYijOld;
00061 extern double DeltaXijNew, DeltaYijNew;
00062 extern double DeltaXij, DeltaYij, DeltaVXij, DeltaVYij;
00063 extern double **DeltaXijOldPair, **DeltaYijOldPair;
00064
00065 //For molecule-ID as per LAMMPS, helpful!
00066 extern int    *molID;
00067 extern int    **isBonded;
```

```
00068
00069 //Following three for MPI only
00070 extern int     *cellList, cells[NDIM+1];
00071 extern int     rank, size, master;
00072 extern double  *fax, *fay, fuSum, fvirSum, frfAtom;
00073
00074 //For thermodynamic properties
00075 extern double  uSumPair, uSumPairPerAtom, virSumPair, virSumPairxx, virSumPairyy, virSumPairxy;
00076 extern double  virSumBond, virSumBondxx, virSumBondyy, virSumBondxy;
00077 extern double  virSumxx, virSumyy, virSumxy;
00078 extern int     freezeAtomType;
00079
00080 // Spacetime Correlations
00081 extern double  **cfOrg, **spacetimeCorr, *cfVal, *spacetimeCorrAv;
00082 extern int     *indexCorr, countCorrAv, limitCorrAv, nBuffCorr, nFunCorr, nValCorr, stepCorr;
00083
00084 // Viscosity
00085 extern double  rfAtom, frfAtom;
00086 extern double  *indexAcf, **viscAcf, *viscAcfOrg, *viscAcfAv, viscAcfInt;
00087 extern int      nValAcf, nBuffAcf, stepAcf, countAcfAv, limitAcfAv;
00088
00089 // Radial distribution function
00090 extern double  *histRdf, rangeRdf;
00091 extern int     countRdf, limitRdf, sizeHistRdf, stepRdf;
00092
00093
00094 // Output files prefixes
00095 extern char    *prefix;
00096
00097 extern char    result[250];
00098 extern FILE    *fpresult;
00099
00100 extern char    xyz[256];
00101 extern FILE    *fpxyz;
00102
00103 extern char    bond[256];
00104 extern FILE    *fpbond;
00105
00106
00107 extern char    dump[256];
00108 extern FILE    *fpdump;
00109
00110 extern char    dnsty[256];
00111 extern FILE    *fpdnsty;
00112
00113 extern char    visc[256];
00114 extern FILE    *fpvisc;
00115
00116 extern char    rdf[256];
00117 extern FILE    *fprdf;
00118
00119 extern char    vrms[256];
00120 extern FILE    *fpvrms;
00121
00122 extern char    stress[256];
00123 extern FILE    *fpstress;
00124
00125 extern char    momentum[256];
00126 extern FILE    *fpmomentum;
00127
00128 extern char    com[256];
00129 extern FILE    *fpcom;
00130
00131 extern char    pair[256];
00132 extern FILE    *fppair;
00133
00134 #endif // GLOBALEXTERN_H
```

3.62 source/Halt.c File Reference

```
#include <stdio.h>
#include <stdlib.h>
#include <stdbool.h>
#include "global.h"
```

Include dependency graph for Halt.c:



Functions

- bool HaltConditionCheck (double value, int stepCount)

3.62.1 Function Documentation

3.62.1.1 HaltConditionCheck()

```
bool HaltConditionCheck (
            double value,
            int stepCount )
```

Definition at line 27 of file Halt.c.

```
00027                                                   {
00028
00029   if(value <= HaltCondition && value != 0) {
00030   fprintf(fpresult, "Halt condition met at step = %d with Vrms = %.10f\n", stepCount, value);
00031   return true;       // Signal that the halt condition is met
00032   }
00033  return false; // Halt condition not met
00034 }
```

References fpresult, HaltCondition, and stepCount.

Referenced by main().

Here is the caller graph for this function:

3.63 Halt.c

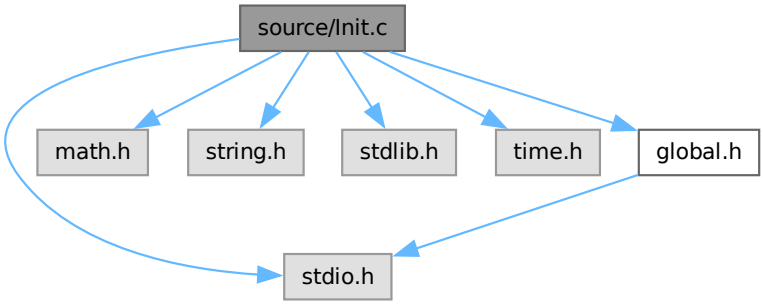
Go to the documentation of this file.

```
00001 /*
00002  * This file is part of Lamina.
00003  *
00004  * Lamina is free software: you can redistribute it and/or modify
00005  * it under the terms of the GNU General Public License as published by
00006  * the Free Software Foundation, either version 3 of the License, or
00007  * (at your option) any later version.
00008  *
00009  * Lamina is distributed in the hope that it will be useful,
00010  * but WITHOUT ANY WARRANTY; without even the implied warranty of
00011  * MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the
00012  * GNU General Public License for more details.
00013  *
00014  * You should have received a copy of the GNU General Public License
00015  * along with Lamina. If not, see <https://www.gnu.org/licenses/>.
00016
00017  Copyright (C) 2025 Harish Charan, University of Durham, UK
00018
00019  */
00020
00021
00022 #include <stdio.h>
00023 #include <stdlib.h>
00024 #include <stdbool.h>
00025 #include "global.h"
00026
00027 bool HaltConditionCheck(double value, int stepCount) {
00028
00029   if(value <= HaltCondition && value != 0) {
00030   fprintf(fpresult, "Halt condition met at step = %d with Vrms = %.10f\n", stepCount, value);
00031   return true;       // Signal that the halt condition is met
00032   }
00033  return false; // Halt condition not met
00034 }
00035
```

3.64 source/Init.c File Reference

```
#include <stdio.h>
#include <math.h>
#include <string.h>
#include <stdlib.h>
#include <time.h>
#include "global.h"
```

Include dependency graph for Init.c:



Functions

- void Init ()

3.64.1 Function Documentation

3.64.1.1 Init()

```
void Init ( )
```

Definition at line 29 of file Init.c.

```
00029           {
00030   char dummy[128];
00031   char inputConfig[128];
00032   FILE *fp;
00033   fp = fopen("input-data","r");
00034   fscanf(fp, "%s %s", dummy, inputConfig);
00035   fscanf(fp, "%s %s", dummy, solver);
00036   fscanf(fp, "%s %s %s", dummy, xBoundary, yBoundary);
00037   fscanf(fp, "%s %d",  dummy, &DampFlag);
00038   fscanf(fp, "%s %d",  dummy, &freezeAtomType);
00039   fscanf(fp, "%s %lf", dummy, &rCut);
00040   fscanf(fp, "%s %lf", dummy, &gamman);
00041   fscanf(fp, "%s %lf", dummy, &kappa);
00042   fscanf(fp, "%s %lf", dummy, &deltaT);
00043   fscanf(fp, "%s %lf", dummy, &strain);
00044   fscanf(fp, "%s %lf", dummy, &FyBylx);
00045   fscanf(fp, "%s %lf", dummy, &fxByfy);
00046   fscanf(fp, "%s %lf", dummy, &DeltaY);
00047   fscanf(fp, "%s %lf", dummy, &DeltaX);
00048   fscanf(fp, "%s %lf", dummy, &HaltCondition);
00049   fscanf(fp, "%s %d",  dummy, &stepAvg);
00050   fscanf(fp, "%s %d",  dummy, &stepEquil);
00051   fscanf(fp, "%s %d",  dummy, &stepLimit);
00052   fscanf(fp, "%s %d",  dummy, &stepDump);
00053   fscanf(fp, "%s %d",  dummy, &stepTraj);
00054   fscanf(fp, "%s %d",  dummy, &limitCorrAv);
00055   fscanf(fp, "%s %d",  dummy, &nBuffCorr);
00056   fscanf(fp, "%s %d",  dummy, &nFunCorr);
00057   fscanf(fp, "%s %d",  dummy, &nValCorr);
00058   fscanf(fp, "%s %d",  dummy, &stepCorr);
00059   fscanf(fp, "%s %d",  dummy, &limitAcfAv);
00060   fscanf(fp, "%s %d",  dummy, &nBuffAcf);
00061   fscanf(fp, "%s %d",  dummy, &nValAcf);
00062   fscanf(fp, "%s %d",  dummy, &stepAcf);
00063   fscanf(fp, "%s %lf", dummy, &rangeRdf);
00064   fscanf(fp, "%s %d",  dummy, &limitRdf);
00065   fscanf(fp, "%s %d",  dummy, &sizeHistRdf);
00066   fscanf(fp, "%s %d",  dummy, &stepRdf);
00067
00068   fclose(fp);
00069   FILE *fpSTATE;
00070   if((fpSTATE = fopen(inputConfig,"r"))==NULL){
00071   printf("Error occurred: Could not open STATE file\n Exiting now..\n");
00072   exit(0);
00073   }
00074
00075   fscanf(fpSTATE, "%s %lf", dummy, &timeNow);
00076   fscanf(fpSTATE, "%s %d",  dummy, &nAtom);
00077   fscanf(fpSTATE, "%s %d",  dummy, &nBond);
00078   fscanf(fpSTATE, "%s %d",  dummy, &nAtomType);
00079   fscanf(fpSTATE, "%s %d",  dummy, &nBondType);
00080   fscanf(fpSTATE, "%s %lf", dummy, &region[1]);
00081   fscanf(fpSTATE, "%s %lf", dummy, &region[2]);
00082
00083   region[2] *= 1.5; //Remove this when put on GitHub
00084
00085   density = nAtom/(region[1]*region[2]);
00086   cells[1] = region[1] / rCut;
00087   cells[2] = region[2] / rCut;
00088   cellList = (int*)malloc((nAtom + cells[1] * cells[2] + 1) * sizeof(int));
00089   regionH[1] = 0.5*region[1];
00090   regionH[2] = 0.5*region[2];
00091
00092   //strain information
00093   strainRate = strain/deltaT;
00094   shearDisplacement = strain * region[2];
00095   shearVelocity = strainRate * region[2];
00096   int n;
```

```
00097
00098   rx = (double*)malloc((nAtom + 1) * sizeof(double));
00099   ry = (double*)malloc((nAtom + 1) * sizeof(double));
00100   vx = (double*)malloc((nAtom + 1) * sizeof(double));
00101   vy = (double*)malloc((nAtom + 1) * sizeof(double));
00102   ax = (double*)malloc((nAtom + 1) * sizeof(double));
00103   ay = (double*)malloc((nAtom + 1) * sizeof(double));
00104   fax = (double*)malloc((nAtom + 1) * sizeof(double));
00105   fay = (double*)malloc((nAtom + 1) * sizeof(double));
00106   atomID = (int*)malloc((nAtom+1) * sizeof(int));
00107   atomType = (int*)malloc((nAtom+1) * sizeof(int));
00108   atomRadius = (double*)malloc((nAtom + 1) * sizeof(double));
00109   atomMass = (double*)malloc((nAtom + 1) * sizeof(double));
00110   speed = (double*)malloc((nAtom + 1) * sizeof(double));
00111   atom1 = (int*)malloc((nBond+1)*sizeof(int));
00112   atom2 = (int*)malloc((nBond+1)*sizeof(int));
00113   BondID = (int*)malloc((nBond+1)*sizeof(int));
00114   BondType = (int*)malloc((nBond+1)*sizeof(int));
00115   kb = (double*)malloc((nBond+1)*sizeof(double));
00116   ro = (double*)malloc((nBond+1)*sizeof(double));
00117   BondEnergy = (double*)malloc((nBond+1)*sizeof(double));
00118   BondLength =(double*)malloc((nBond+1)*sizeof(double));
00119   discDragx = (double*)malloc((nAtom + 1) * sizeof(double));
00120   discDragy = (double*)malloc((nAtom + 1) * sizeof(double));
00121   nodeDragx = (double*)malloc((nAtom + 1) * sizeof(double));
00122   nodeDragy = (double*)malloc((nAtom + 1) * sizeof(double));
00123   ImageX = (int*)malloc((nAtom+1) * sizeof(int));
00124   ImageY = (int*)malloc((nAtom+1) * sizeof(int));
00125   rxUnwrap = (double*)malloc((nAtom + 1) * sizeof(double));
00126   ryUnwrap = (double*)malloc((nAtom + 1) * sizeof(double));
00127   DeltaXijOld = (double*)malloc((nBond+1)*sizeof(double));
00128   DeltaYijOld = (double*)malloc((nBond+1)*sizeof(double));
00129   DeltaXijOldPair = (double**)malloc((nAtom+1) * sizeof(double*));
00130   DeltaYijOldPair = (double**)malloc((nAtom+1) * sizeof(double*));
00131   for(int n = 0; n <= nAtom; n++) {
00132    DeltaXijOldPair[n] = (double*)malloc((nAtom+1) * sizeof(double));
00133    DeltaYijOldPair[n] = (double*)malloc((nAtom+1) * sizeof(double));
00134   }
00135   molID = (int*)malloc((nAtom+1) * sizeof(int));
00136
00137   for(n = 1; n <= nAtom; n ++){
00138    atomMass[n] = 1.0;
00139   }
00140
00141   fscanf(fpSTATE, "%s\n", dummy);
00142   for(n = 1; n <= nAtom; n ++)
00143    fscanf(fpSTATE, "%d %d %d %lf %lf %lf %lf %lf\n", &atomID[n], &molID[n], &atomType[n],
      &atomRadius[n], &rx[n], &ry[n], &vx[n], &vy[n]);
00144
00145
00146   fscanf(fpSTATE, "%s\n", dummy);
00147   for(n=1; n<=nBond; n++)
00148    fscanf(fpSTATE, "%d %d %d %d %lf %lf\n", &BondID[n], &BondType[n], &atom1[n], &atom2[n], &kb[n],
      &ro[n]);
00149
00150   fclose(fpSTATE);
00151
00152  //2D-List of bonded atoms. This is used to remove pair interaction
00153  //calculation for the bonded atoms
00154    isBonded = (int**)malloc((nAtom + 1) * sizeof(int*));
00155   for (int i = 0; i <= nAtom; i++) {
00156     isBonded[i] = (int*)malloc((nAtom + 1) * sizeof(int));
00157     for (int j = 0; j <= nAtom; j++) {
00158         isBonded[i][j] = 0;
00159     }
00160   }
00161
00162   for (n = 1; n <= nBond; n++) {
00163     int i = atom1[n];
00164     int j = atom2[n];
00165     isBonded[i][j] = 1;
00166     isBonded[j][i] = 1; // symmetric
00167 }
00168
00169  //For thermostate, update in final version
00170 thermo = 'C';
00171
00172
00173  // List the interface atoms
00174  nAtomInterface = 0;
00175  nAtomBlock = 0;
00176  nDiscInterface = 0;
00177  double InterfaceWidth, bigDiameter;
00178  bigDiameter = 2.8;
00179  InterfaceWidth = 5.0 * bigDiameter;
00180
00181  for(n = 1; n <= nAtom; n++){
```

```
00182   if(fabs(ry[n]) < InterfaceWidth){
00183   nAtomInterface++;
00184   }
00185   if(molID[n] == 2){
00186   nAtomBlock++;
00187   }
00188   if(atomRadius[n] != 0.0){
00189   nDiscInterface++;
00190   } }
00191
00192    atomIDInterface =  (int*)malloc((nAtomInterface+1)*sizeof(int));
00193
00194   int m;
00195   m = 1;
00196   for(n=1; n<=nAtom; n++){
00197    if(fabs(ry[n]) < InterfaceWidth){
00198    atomIDInterface[m] = atomID[n];
00199    m++;
00200    } }
00201
00202   nPairTotal = 0.5 * nAtomInterface * (nAtomInterface-1);
00203   PairID = (int*)malloc((nPairTotal+1) * sizeof(int));
00204   Pairatom1 = (int*)malloc((nPairTotal+1) * sizeof(int));
00205   Pairatom2 = (int*)malloc((nPairTotal+1) * sizeof(int));
00206   PairXij = (double*)malloc((nPairTotal+1) * sizeof(double));
00207   PairYij = (double*)malloc((nPairTotal+1) * sizeof(double));
00208
00209     fprintf(fpresult, "-----------------------------------\n");
00210     fprintf(fpresult, "-------PARAMETERS-----------\n");
00211     fprintf(fpresult, "-----------------------------------\n");
00212     fprintf(fpresult, "nAtom\t\t\t%d\n",  nAtom);
00213     fprintf(fpresult, "nBond\t\t\t%d\n",  nBond);
00214     fprintf(fpresult, "nAtomBlock\t\t%d\n",  nAtomBlock);
00215     fprintf(fpresult, "nAtomInterface\t%d\n",  nAtomInterface);
00216     fprintf(fpresult, "nDiscInterface\t\t%d\n",  nDiscInterface);
00217     fprintf(fpresult, "gamman\t\t\t%0.6g\n", gamman);
00218     fprintf(fpresult, "strain\t\t\t%0.6g\n", strain);
00219     fprintf(fpresult, "strainRate\t\t%0.6g\n", strainRate);
00220     fprintf(fpresult, "FyBylx\t\t\t%0.6g\n", FyBylx);
00221     fprintf(fpresult, "fxByfy\t\t\t%0.6g\n", fxByfy);
00222     fprintf(fpresult, "DeltaY\t\t\t%0.6g\n", DeltaY);
00223     fprintf(fpresult, "DeltaX\t\t\t%0.6g\n", DeltaX);
00224     fprintf(fpresult, "HaltCondition\t\t%0.6g\n", HaltCondition);
00225     fprintf(fpresult, "kappa\t\t\t%g\n", kappa);
00226     fprintf(fpresult, "density\t\t\t%g\n", density);
00227     fprintf(fpresult, "rCut\t\t\t\t%g\n", rCut);
00228     fprintf(fpresult, "deltaT\t\t\t%g\n", deltaT);
00229     fprintf(fpresult, "stepEquil\t\t\t%d\n",  stepEquil);
00230     fprintf(fpresult, "stepLimit\t\t\t%d\n",  stepLimit);
00231     fprintf(fpresult, "region[1]\t\t\t%0.16lf\n", region[1]);
00232     fprintf(fpresult, "region[2]\t\t\t%0.16lf\n", region[2]);
00233     fprintf(fpresult, "cells[1]\t\t\t%d\n",  cells[1]);
00234     fprintf(fpresult, "cells[2]\t\t\t%d\n",  cells[2]);
00235     fprintf(fpresult, "solver\t\t\t%s\n",  solver);
00236     fprintf(fpresult, "boundary\t\t\t%s %s\n", xBoundary, yBoundary);
00237     fprintf(fpresult, "DampFlag\t\t%d\n",  DampFlag);
00238
00239
00240     fprintf(fpresult, "-----------------------------------\n");
00241     fprintf(fpresult, "#TimeNow TotalMomentum PotEngyPerAtom KinEngyPerAtom TotEngyPerAtom
    PairEnergyPerAtom BondEnergyPerAtom  Press VirialSum\n");
00242     fprintf(fpvrms, "#timeNow\tVrms \n");
00243     fprintf(fpcom, "#timeNow\tComX\tComY\n");
00244
00245 /* //Uncomment the following as per your acquirement
00246     fprintf(fpstress, "strain          %lf\n", strain);
00247     fprintf(fpstress, "region[1]       %lf\n", region[1]);
00248     fprintf(fpstress, "region[2]       %lf\n", region[2]);
00249     fprintf(fpstress, "#timeNow virSumxx virSumyy virSumxy pressure\n");
00250     fprintf(fpmomentum, "#timeNow Px Py\n");
00251 */
00252
00253    if((strcmp(xBoundary, "p") != 0 && strcmp(xBoundary, "r") != 0) ||
00254     (strcmp(yBoundary, "p") != 0 && strcmp(yBoundary, "r") != 0)) {
00255     fprintf(fpresult, "Error: Invalid boundary value detected: '%s %s'. Only 'p' or 'r' are
    allowed.\n", xBoundary, yBoundary);
00256     exit(EXIT_FAILURE); // Exit with failure status
00257   }
00258
00259 }
```

References atom1, atom2, atomID, atomIDInterface, atomMass, atomRadius, atomType, ax, ay, BondEnergy, BondID, BondLength, BondType, cellList, cells, DampFlag, deltaT, DeltaX, DeltaXijOld, DeltaXijOldPair, DeltaY, DeltaYijOld, DeltaYijOldPair, density, discDragx, discDragy, fax, fay, fpcom, fpresult, fpvrms, freezeAtomType, fxByfy, FyBylx, gamman, HaltCondition, ImageX, ImageY, isBonded, kappa, kb, limitAcfAv, limitCorrAv, limitRdf,

molID, nAtom, nAtomBlock, nAtomInterface, nAtomType, nBond, nBondType, nBuffAcf, nBuffCorr, nDiscInterface, nFunCorr, nodeDragx, nodeDragy, nPairTotal, nValAcf, nValCorr, Pairatom1, Pairatom2, PairID, PairXij, PairYij, rangeRdf, rCut, region, regionH, ro, rx, rxUnwrap, ry, ryUnwrap, shearDisplacement, shearVelocity, sizeHistRdf, solver, speed, stepAcf, stepAvg, stepCorr, stepDump, stepEquil, stepLimit, stepRdf, stepTraj, strain, strainRate, thermo, timeNow, vx, vy, xBoundary, and yBoundary.

Referenced by main().

Here is the caller graph for this function:

3.65 Init.c

Go to the documentation of this file.

```
00001 /*
00002  * This file is part of Lamina.
00003  *
00004  * Lamina is free software: you can redistribute it and/or modify
00005  * it under the terms of the GNU General Public License as published by
00006  * the Free Software Foundation, either version 3 of the License, or
00007  * (at your option) any later version.
00008  *
00009  * Lamina is distributed in the hope that it will be useful,
00010  * but WITHOUT ANY WARRANTY; without even the implied warranty of
00011  * MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the
00012  * GNU General Public License for more details.
00013  *
00014  * You should have received a copy of the GNU General Public License
00015  * along with Lamina. If not, see <https://www.gnu.org/licenses/>.
00016
00017  Copyright (C) 2025 Harish Charan, University of Durham, UK
00018
00019  */
00020
00021
00022 #include<stdio.h>
00023 #include<math.h>
00024 #include<string.h>
00025 #include<stdlib.h>
00026 #include <time.h>
00027 #include"global.h"
00028
00029 void Init(){
00030   char dummy[128];
00031   char inputConfig[128];
00032   FILE *fp;
00033   fp = fopen("input-data","r");
00034   fscanf(fp, "%s %s", dummy, inputConfig);
00035   fscanf(fp, "%s %s", dummy, solver);
00036   fscanf(fp, "%s %s %s", dummy, xBoundary, yBoundary);
00037   fscanf(fp, "%s %d",  dummy, &DampFlag);
00038   fscanf(fp, "%s %d",  dummy, &freezeAtomType);
00039   fscanf(fp, "%s %lf", dummy, &rCut);
00040   fscanf(fp, "%s %lf", dummy, &gamman);
00041   fscanf(fp, "%s %lf", dummy, &kappa);
00042   fscanf(fp, "%s %lf", dummy, &deltaT);
00043   fscanf(fp, "%s %lf", dummy, &strain);
00044   fscanf(fp, "%s %lf", dummy, &FyBylx);
00045   fscanf(fp, "%s %lf", dummy, &fxByfy);
00046   fscanf(fp, "%s %lf", dummy, &DeltaY);
00047   fscanf(fp, "%s %lf", dummy, &DeltaX);
00048   fscanf(fp, "%s %lf", dummy, &HaltCondition);
00049   fscanf(fp, "%s %d",  dummy, &stepAvg);
```

```
00050   fscanf(fp, "%s %d",  dummy, &stepEquil);
00051   fscanf(fp, "%s %d",  dummy, &stepLimit);
00052   fscanf(fp, "%s %d",  dummy, &stepDump);
00053   fscanf(fp, "%s %d",  dummy, &stepTraj);
00054   fscanf(fp, "%s %d",  dummy, &limitCorrAv);
00055   fscanf(fp, "%s %d",  dummy, &nBuffCorr);
00056   fscanf(fp, "%s %d",  dummy, &nFunCorr);
00057   fscanf(fp, "%s %d",  dummy, &nValCorr);
00058   fscanf(fp, "%s %d",  dummy, &stepCorr);
00059   fscanf(fp, "%s %d",  dummy, &limitAcfAv);
00060   fscanf(fp, "%s %d",  dummy, &nBuffAcf);
00061   fscanf(fp, "%s %d",  dummy, &nValAcf);
00062   fscanf(fp, "%s %d",  dummy, &stepAcf);
00063   fscanf(fp, "%s %lf", dummy, &rangeRdf);
00064   fscanf(fp, "%s %d",  dummy, &limitRdf);
00065   fscanf(fp, "%s %d",  dummy, &sizeHistRdf);
00066   fscanf(fp, "%s %d",  dummy, &stepRdf);
00067
00068   fclose(fp);
00069   FILE *fpSTATE;
00070   if((fpSTATE = fopen(inputConfig,"r"))==NULL){
00071   printf("Error occurred: Could not open STATE file\n Exiting now..\n");
00072   exit(0);
00073   }
00074
00075   fscanf(fpSTATE, "%s %lf", dummy, &timeNow);
00076   fscanf(fpSTATE, "%s %d",  dummy, &nAtom);
00077   fscanf(fpSTATE, "%s %d",  dummy, &nBond);
00078   fscanf(fpSTATE, "%s %d",  dummy, &nAtomType);
00079   fscanf(fpSTATE, "%s %d",  dummy, &nBondType);
00080   fscanf(fpSTATE, "%s %lf", dummy, &region[1]);
00081   fscanf(fpSTATE, "%s %lf", dummy, &region[2]);
00082
00083   region[2] *= 1.5; //Remove this when put on GitHub
00084
00085   density = nAtom/(region[1]*region[2]);
00086   cells[1] = region[1] / rCut;
00087   cells[2] = region[2] / rCut;
00088   cellList = (int*)malloc((nAtom + cells[1] * cells[2] + 1) * sizeof(int));
00089   regionH[1] = 0.5*region[1];
00090   regionH[2] = 0.5*region[2];
00091
00092   //strain information
00093   strainRate = strain/deltaT;
00094   shearDisplacement = strain * region[2];
00095   shearVelocity = strainRate * region[2];
00096   int n;
00097
00098   rx = (double*)malloc((nAtom + 1) * sizeof(double));
00099   ry = (double*)malloc((nAtom + 1) * sizeof(double));
00100   vx = (double*)malloc((nAtom + 1) * sizeof(double));
00101   vy = (double*)malloc((nAtom + 1) * sizeof(double));
00102   ax = (double*)malloc((nAtom + 1) * sizeof(double));
00103   ay = (double*)malloc((nAtom + 1) * sizeof(double));
00104   fax = (double*)malloc((nAtom + 1) * sizeof(double));
00105   fay = (double*)malloc((nAtom + 1) * sizeof(double));
00106   atomID = (int*)malloc((nAtom+1) * sizeof(int));
00107   atomType = (int*)malloc((nAtom+1) * sizeof(int));
00108   atomRadius = (double*)malloc((nAtom + 1) * sizeof(double));
00109   atomMass = (double*)malloc((nAtom + 1) * sizeof(double));
00110   speed = (double*)malloc((nAtom + 1) * sizeof(double));
00111   atom1 = (int*)malloc((nBond+1)*sizeof(int));
00112   atom2 = (int*)malloc((nBond+1)*sizeof(int));
00113   BondID = (int*)malloc((nBond+1)*sizeof(int));
00114   BondType = (int*)malloc((nBond+1)*sizeof(int));
00115   kb = (double*)malloc((nBond+1)*sizeof(double));
00116   ro = (double*)malloc((nBond+1)*sizeof(double));
00117   BondEnergy = (double*)malloc((nBond+1)*sizeof(double));
00118   BondLength =(double*)malloc((nBond+1)*sizeof(double));
00119   discDragx = (double*)malloc((nAtom + 1) * sizeof(double));
00120   discDragy = (double*)malloc((nAtom + 1) * sizeof(double));
00121   nodeDragx = (double*)malloc((nAtom + 1) * sizeof(double));
00122   nodeDragy = (double*)malloc((nAtom + 1) * sizeof(double));
00123   ImageX = (int*)malloc((nAtom+1) * sizeof(int));
00124   ImageY = (int*)malloc((nAtom+1) * sizeof(int));
00125   rxUnwrap = (double*)malloc((nAtom + 1) * sizeof(double));
00126   ryUnwrap = (double*)malloc((nAtom + 1) * sizeof(double));
00127   DeltaXijOld = (double*)malloc((nBond+1)*sizeof(double));
00128   DeltaYijOld = (double*)malloc((nBond+1)*sizeof(double));
00129   DeltaXijOldPair = (double**)malloc((nAtom+1) * sizeof(double*));
00130   DeltaYijOldPair = (double**)malloc((nAtom+1) * sizeof(double*));
00131   for(int n = 0; n <= nAtom; n++) {
00132    DeltaXijOldPair[n] = (double*)malloc((nAtom+1) * sizeof(double));
00133    DeltaYijOldPair[n] = (double*)malloc((nAtom+1) * sizeof(double));
00134   }
00135   molID = (int*)malloc((nAtom+1) * sizeof(int));
00136
```

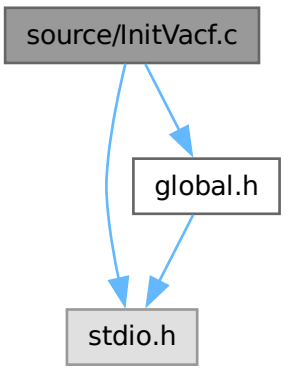
```
00137   for(n = 1; n <= nAtom; n ++){
00138    atomMass[n] = 1.0;
00139   }
00140
00141   fscanf(fpSTATE, "%s\n", dummy);
00142   for(n = 1; n <= nAtom; n ++)
00143    fscanf(fpSTATE, "%d %d %d %lf %lf %lf %lf %lf\n", &atomID[n], &molID[n], &atomType[n],
      &atomRadius[n], &rx[n], &ry[n], &vx[n], &vy[n]);
00144
00145
00146   fscanf(fpSTATE, "%s\n", dummy);
00147   for(n=1; n<=nBond; n++)
00148    fscanf(fpSTATE, "%d %d %d %d %lf %lf\n", &BondID[n], &BondType[n], &atom1[n], &atom2[n], &kb[n],
      &ro[n]);
00149
00150   fclose(fpSTATE);
00151
00152  //2D-List of bonded atoms. This is used to remove pair interaction
00153  //calculation for the bonded atoms
00154    isBonded = (int**)malloc((nAtom + 1) * sizeof(int*));
00155   for (int i = 0; i <= nAtom; i++) {
00156     isBonded[i] = (int*)malloc((nAtom + 1) * sizeof(int));
00157     for (int j = 0; j <= nAtom; j++) {
00158         isBonded[i][j] = 0;
00159     }
00160   }
00161
00162   for (n = 1; n <= nBond; n++) {
00163     int i = atom1[n];
00164     int j = atom2[n];
00165     isBonded[i][j] = 1;
00166     isBonded[j][i] = 1; // symmetric
00167 }
00168
00169  //For thermostate, update in final version
00170 thermo = 'C';
00171
00172
00173  // List the interface atoms
00174  nAtomInterface = 0;
00175  nAtomBlock = 0;
00176  nDiscInterface = 0;
00177  double InterfaceWidth, bigDiameter;
00178  bigDiameter = 2.8;
00179  InterfaceWidth = 5.0 * bigDiameter;
00180
00181  for(n = 1; n <= nAtom; n++){
00182   if(fabs(ry[n]) < InterfaceWidth){
00183   nAtomInterface++;
00184   }
00185   if(molID[n] == 2){
00186   nAtomBlock++;
00187   }
00188   if(atomRadius[n] != 0.0){
00189   nDiscInterface++;
00190   } }
00191
00192    atomIDInterface =  (int*)malloc((nAtomInterface+1)*sizeof(int));
00193
00194   int m;
00195   m = 1;
00196   for(n=1; n<=nAtom; n++){
00197    if(fabs(ry[n]) < InterfaceWidth){
00198    atomIDInterface[m] = atomID[n];
00199    m++;
00200    } }
00201
00202   nPairTotal = 0.5 * nAtomInterface * (nAtomInterface-1);
00203   PairID = (int*)malloc((nPairTotal+1) * sizeof(int));
00204   Pairatom1 = (int*)malloc((nPairTotal+1) * sizeof(int));
00205   Pairatom2 = (int*)malloc((nPairTotal+1) * sizeof(int));
00206   PairXij = (double*)malloc((nPairTotal+1) * sizeof(double));
00207   PairYij = (double*)malloc((nPairTotal+1) * sizeof(double));
00208
00209     fprintf(fpresult, "-------------------------------------\n");
00210     fprintf(fpresult, "-------PARAMETERS-----------\n");
00211     fprintf(fpresult, "-------------------------------------\n");
00212     fprintf(fpresult, "nAtom\t\t\t%d\n",  nAtom);
00213     fprintf(fpresult, "nBond\t\t\t%d\n",  nBond);
00214     fprintf(fpresult, "nAtomBlock\t\t%d\n",  nAtomBlock);
00215     fprintf(fpresult, "nAtomInterface\t%d\n",  nAtomInterface);
00216     fprintf(fpresult, "nDiscInterface\t\t%d\n",  nDiscInterface);
00217     fprintf(fpresult, "gamman\t\t\t%0.6g\n", gamman);
00218     fprintf(fpresult, "strain\t\t\t%0.6g\n", strain);
00219     fprintf(fpresult, "strainRate\t\t%0.6g\n", strainRate);
00220     fprintf(fpresult, "FyBylx\t\t\t%0.6g\n", FyBylx);
00221     fprintf(fpresult, "fxByfy\t\t\t%0.6g\n", fxByfy);
```

```
00222     fprintf(fpresult, "DeltaY\t\t\t%0.6g\n", DeltaY);
00223     fprintf(fpresult, "DeltaX\t\t\t%0.6g\n", DeltaX);
00224     fprintf(fpresult, "HaltCondition\t\t%0.6g\n", HaltCondition);
00225     fprintf(fpresult, "kappa\t\t\t%g\n", kappa);
00226     fprintf(fpresult, "density\t\t\t%g\n", density);
00227     fprintf(fpresult, "rCut\t\t\t\t%g\n", rCut);
00228     fprintf(fpresult, "deltaT\t\t\t%g\n", deltaT);
00229     fprintf(fpresult, "stepEquil\t\t\t%d\n",  stepEquil);
00230     fprintf(fpresult, "stepLimit\t\t\t%d\n",  stepLimit);
00231     fprintf(fpresult, "region[1]\t\t\t%0.16lf\n", region[1]);
00232     fprintf(fpresult, "region[2]\t\t\t%0.16lf\n", region[2]);
00233     fprintf(fpresult, "cells[1]\t\t\t%d\n",  cells[1]);
00234     fprintf(fpresult, "cells[2]\t\t\t%d\n",  cells[2]);
00235     fprintf(fpresult, "solver\t\t\t%s\n",  solver);
00236     fprintf(fpresult, "boundary\t\t\t%s %s\n", xBoundary, yBoundary);
00237     fprintf(fpresult, "DampFlag\t\t%d\n",  DampFlag);
00238
00239
00240     fprintf(fpresult, "-------------------------------------\n");
00241     fprintf(fpresult, "#TimeNow TotalMomentum PotEngyPerAtom KinEngyPerAtom TotEngyPerAtom
      PairEnergyPerAtom BondEnergyPerAtom  Press VirialSum\n");
00242     fprintf(fpvrms, "#timeNow\tVrms \n");
00243     fprintf(fpcom, "#timeNow\tComX\tComY\n");
00244
00245 /* //Uncomment the following as per your acquirement
00246     fprintf(fpstress, "strain           %lf\n", strain);
00247     fprintf(fpstress, "region[1]        %lf\n", region[1]);
00248     fprintf(fpstress, "region[2]        %lf\n", region[2]);
00249     fprintf(fpstress, "#timeNow virSumxx virSumyy virSumxy pressure\n");
00250     fprintf(fpmomentum, "#timeNow Px Py\n");
00251 */
00252
00253    if((strcmp(xBoundary, "p") != 0 && strcmp(xBoundary, "r") != 0) ||
00254     (strcmp(yBoundary, "p") != 0 && strcmp(yBoundary, "r") != 0)) {
00255     fprintf(fpresult, "Error: Invalid boundary value detected: '%s %s'. Only 'p' or 'r' are
      allowed.\n", xBoundary, yBoundary);
00256     exit(EXIT_FAILURE); // Exit with failure status
00257   }
00258
00259 }
```

3.66 source/InitVacf.c File Reference

```
#include <stdio.h>
#include "global.h"
```

Include dependency graph for InitVacf.c:



Functions

- void ZeroVacf ()
- void InitVacf ()

3.66.1 Function Documentation

3.66.1.1 InitVacf()

```
void InitVacf ( )
```

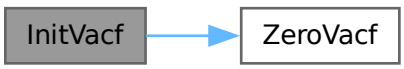
Definition at line 26 of file InitVacf.c.

```
00026                {
00027   int nb;
00028   for(nb = 1 ; nb <= nBuffAcf ; nb ++)
00029     indexAcf[nb] = -(nb-1)*nValAcf/nBuffAcf;
00030   ZeroVacf();
00031 }
```

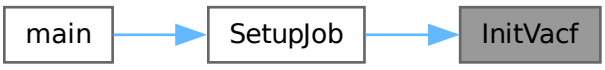
References indexAcf, nBuffAcf, nValAcf, and ZeroVacf().

Referenced by SetupJob().

Here is the call graph for this function:



Here is the caller graph for this function:



3.66.1.2 ZeroVacf()

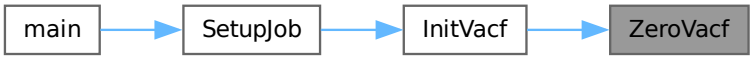
```
void ZeroVacf ( )
```

Definition at line 25 of file ZeroVacf.c.

```
00025                {
00026  int j;
00027  countAcfAv= 0 ;
00028  for(j = 1 ; j <= nValAcf ; j ++)
00029   viscAcfAv[j] = 0.;
00030 }
```

Referenced by InitVacf().

Here is the caller graph for this function:



3.67 InitVacf.c

Go to the documentation of this file.

```
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00008  *
00009  * Lamina is distributed in the hope that it will be useful,
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00014  * You should have received a copy of the GNU General Public License
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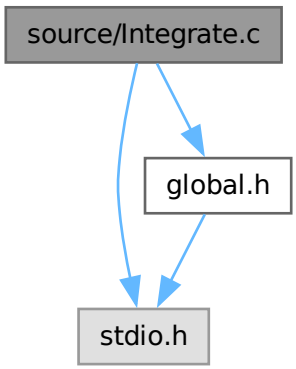
00016
00017  Copyright (C) 2025 Harish Charan, University of Durham, UK
00018
00019  */
00020
00021
00022 #include<stdio.h>
00023 #include"global.h"
00024
00025 void ZeroVacf();
00026 void InitVacf(){
00027   int nb;
00028   for(nb = 1 ; nb <= nBuffAcf ; nb ++)
00029     indexAcf[nb] = -(nb-1)*nValAcf/nBuffAcf;
00030   ZeroVacf();
00031 }
```

3.68 source/Integrate.c File Reference

```
#include <stdio.h>
#include "global.h"
```

Include dependency graph for Integrate.c:



Functions

- double Integrate (double *f, int nf)

3.68.1 Function Documentation

3.68.1.1 Integrate()

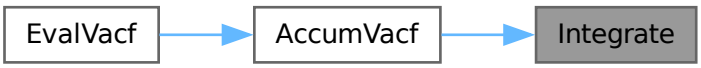
```
double Integrate (
            double * f,
            int nf )
```

Definition at line 25 of file Integrate.c.

```
00025                                   {
00026  double s;
00027  int i;
00028  s = 0.5*(f[1] + f[nf]);
00029  for(i = 2 ; i <= nf - 1 ; i ++)
00030   s += f[i];
00031  return(s);
00032 }
```

Referenced by AccumVacf().

Here is the caller graph for this function:



3.69 Integrate.c

Go to the documentation of this file.

```
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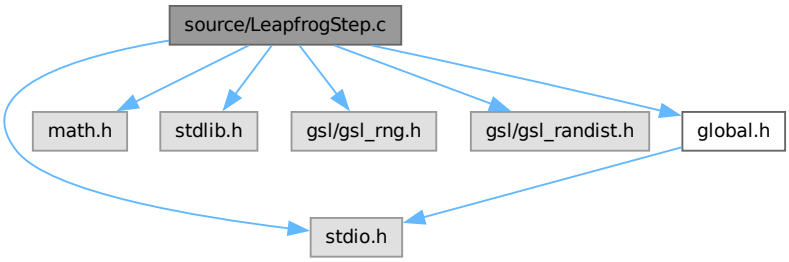
00016
00017  Copyright (C) 2025 Harish Charan, University of Durham, UK
00018
00019  */
00020
00021
00022 #include<stdio.h>
00023 #include"global.h"
00024
00025 double Integrate(double *f, int nf){
00026  double s;
00027  int i;
00028  s = 0.5*(f[1] + f[nf]);
00029  for(i = 2 ; i <= nf - 1 ; i ++)
00030   s += f[i];
00031  return(s);
00032 }
00033
```

3.70 source/LeapfrogStep.c File Reference

```
#include <stdio.h>
#include <math.h>
#include <stdlib.h>
#include <gsl/gsl_rng.h>
#include <gsl/gsl_randist.h>
#include "global.h"
```

Include dependency graph for LeapfrogStep.c:



Functions

- void LeapfrogStep (char thermo, gsl_rng *rnd)

3.70.1 Function Documentation

3.70.1.1 LeapfrogStep()

```
void LeapfrogStep (
            char thermo,
            gsl_rng * rnd )
```

Definition at line 28 of file LeapfrogStep.c.

```
00028                                                {
00029 double temperature, GAMMA;
00030 GAMMA = 100;
00031
00032 double *TValSum;
00033 TValSum = (double*)malloc((nAtom + 1) * sizeof(double));
00034
00035
00036   if(stepCount <= stepEquil){
00037     double gSum, varS, massS;
00038     temperature = 1./GAMMA;
00039
00040    if(stepCount == 1) varS = 0.;
00041     double A, S1, S2, T;
00042     int n;
00043     S1 = 0.; S2 = 0.; gSum = 0.; massS = 0.1;
00044
00045     vvSum = 0.;
00046     double halfdt = 0.5*deltaT;
00047     for (n = 1; n <= nAtom; n++){
00048       T = vx[n] + halfdt * ax[n];
00049       S1 += T * ax[n];
00050       S2 += Sqr(T);
00051
00052       T = vy[n] + halfdt * ay[n];
00053       S1 += T * ay[n];
00054       S2 += Sqr(T);
00055      vvSum += (Sqr(vx[n]) +  Sqr(vy[n]));
00056     }
00057
00058     A = -S1 / S2;
00059     S2 = vvSum;
00060
00061     double C = 1 + A*deltaT ;
00062     double D = deltaT * (1 + 0.5 * A * deltaT);
00063
00064     int i,j;
00065     real dr[NDIM+1], r, rr, ri, rrCut;
00066     double vv;
00067
00068     double uVal, AA, AASum;
00069     double TVal;
00070
00071     double deno, VVSum;
00072     deno = 0.;
00073     VVSum = 0.;
00074     AASum = 0.;
00075
00076   for(n=1;n<=nAtom; n++)
00077      TValSum[n] = 0.;
00078
00079   rrCut = Sqr(rCut);
00080
00081 /*****Calculating Configarational temperature*****/
00082 //Solving the equation of motion here
00083 if(thermo == 'C'){
00084 for(i = 1 ; i <= nAtom; i ++){
00085     for(j = i+1 ; j <= nAtom ; j ++){
00086       dr[1] = rx[i] - rx[j];
00087       if(fabs(dr[1]) > regionH[1])
00088     dr[1] -= SignR(region[1], dr[1]);
00089
00090      dr[2] = ry[i] - ry[j];
00091       if(fabs(dr[2]) > regionH[2])
00092     dr[2] -= SignR(region[2], dr[2]);
00093
00094      rr = Sqr(dr[1]) + Sqr(dr[2]);
00095      if(rr < rrCut ){
00096      r = sqrt(rr);
00097      ri = 1/r;
00098      uVal = ri*exp(-kappa*r);
00099
00100      TVal = (1./rr + Sqr(kappa) + kappa/r)*uVal;
```

```
00101       TValSum[i] += TVal;
00102       TValSum[j] += TVal;
00103     } }
00104       AA = Sqr(ax[i]) + Sqr(ay[i]);
00105       AASum += AA;
00106       vv = Sqr(vx[i]) + Sqr(vy[i]);
00107       VVSum += vv;
00108       deno += TValSum[i];
00109 }
00110
00111       double gSumconfig, varSconfig, massSconfig;
00112       if(stepCount == 1) varSconfig = 0.;
00113       gSumconfig = 0.; massSconfig = 2.0;
00114
00115       gSumconfig = (AASum/temperature - deno)/massSconfig;
00116       varSconfig += deltaT*gSumconfig;
00117
00118        /*****Configarational Nose-Hoover thermostat*****/
00119     for (n = 1; n <= nAtom; n++){
00120        vx[n] += deltaT * ax[n];
00121        rx[n] += deltaT * (vx[n] + varSconfig * ax[n]);
00122        vy[n] += deltaT * ay[n];
00123        ry[n] += deltaT * (vy[n] + varSconfig * ay[n]);
00124      }
00125        /*****Kinetic Nose-Hoover thermostat*****/
00126    }else if(thermo == 'N'){
00127      gSum = (0.5*S2 - (nAtom + 1)*temperature)/massS;
00128      varS += deltaT*gSum;
00129     for (n = 1; n <= nAtom; n++){
00130        vx[n] += deltaT * (ax[n] - varS *vx[n]);
00131        rx[n] += deltaT * vx[n];
00132        vy[n] += deltaT * (ay[n] - varS *vy[n]);
00133        ry[n] += deltaT * vy[n];
00134     }
00135        /*****for Gaussian thermostat*****/
00136   }else if(thermo == 'G'){
00137        for (n = 1; n <= nAtom; n++){
00138        vx[n] = C * vx[n] + D * ax[n];
00139        rx[n] += deltaT * vx[n];
00140        vy[n] = C * vy[n] + D * ay[n];
00141        ry[n] += deltaT * vy[n];
00142       }
00143    }else if (thermo == 'L'){
00144    double nu = 0.03066;
00145    double var = sqrt(2*nu/(GAMMA*deltaT));
00146    double scale = 1. + nu*deltaT/2.;
00147    double scale_v = 2./scale - 1.;
00148    double scale_f = deltaT/scale;
00149    int n;
00150    for(n = 1 ; n <= nAtom ; n ++){
00151        vx[n] = scale_v*vx[n] + scale_f*(ax[n] + var*gsl_ran_gaussian(rnd,1));
00152        rx[n] += deltaT * vx[n];
00153        vy[n] = scale_v*vy[n] + scale_f*(ay[n] + var*gsl_ran_gaussian(rnd,1));
00154        ry[n] += deltaT * vy[n];
00155      }
00156    }
00157   }else{
00158      int n;
00159      for(n = 1 ; n <= nAtom ; n ++){
00160        vx[n] += deltaT * ax[n];
00161        rx[n] += deltaT * vx[n];
00162        vy[n] += deltaT * ay[n];
00163        ry[n] += deltaT * vy[n];
00164      }
00165    }
00166 }
```

References ax, ay, deltaT, kappa, nAtom, NDIM, rCut, region, regionH, rx, ry, SignR, Sqr, stepCount, stepEquil, thermo, vvSum, vx, and vy.

3.71 LeapfrogStep.c

Go to the documentation of this file.

```
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00007  * (at your option) any later version.
```

```
00008  *
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00011  * MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the
00012  * GNU General Public License for more details.
00013  *
00014  * You should have received a copy of the GNU General Public License
00015  * along with Lamina. If not, see <https://www.gnu.org/licenses/>.
00016
00017  Copyright (C) 2025 Harish Charan, University of Durham, UK
00018
00019  */
00020 #include<stdio.h>
00021 #include<math.h>
00022 #include<stdlib.h>
00023 #include <gsl/gsl_rng.h>
00024 #include <gsl/gsl_randist.h>
00025 #include"global.h"
00026
00027
00028 void LeapfrogStep(char thermo, gsl_rng * rnd){
00029 double temperature, GAMMA;
00030 GAMMA = 100;
00031
00032 double *TValSum;
00033 TValSum = (double*)malloc((nAtom + 1) * sizeof(double));
00034
00035
00036   if(stepCount <= stepEquil){
00037     double gSum, varS, massS;
00038     temperature = 1./GAMMA;
00039
00040    if(stepCount == 1) varS = 0.;
00041     double A, S1, S2, T;
00042     int n;
00043     S1 = 0.; S2 = 0.; gSum = 0.; massS = 0.1;
00044
00045     vvSum = 0.;
00046     double halfdt = 0.5*deltaT;
00047     for (n = 1; n <= nAtom; n++){
00048       T = vx[n] + halfdt * ax[n];
00049       S1 += T * ax[n];
00050       S2 += Sqr(T);
00051
00052       T = vy[n] + halfdt * ay[n];
00053       S1 += T * ay[n];
00054       S2 += Sqr(T);
00055      vvSum += (Sqr(vx[n]) +  Sqr(vy[n]));
00056     }
00057
00058     A = -S1 / S2;
00059     S2 = vvSum;
00060
00061     double C = 1 + A*deltaT ;
00062     double D = deltaT * (1 + 0.5 * A * deltaT);
00063
00064     int i,j;
00065     real dr[NDIM+1], r, rr, ri, rrCut;
00066     double vv;
00067
00068     double uVal, AA, AASum;
00069     double TVal;
00070
00071     double deno, VVSum;
00072     deno = 0.;
00073     VVSum = 0.;
00074     AASum = 0.;
00075
00076   for(n=1;n<=nAtom; n++)
00077      TValSum[n] = 0.;
00078
00079   rrCut = Sqr(rCut);
00080
00081 /*****Calculating Configarational temperature*****/
00082 //Solving the equation of motion here
00083 if(thermo == 'C'){
00084 for(i = 1 ; i <= nAtom; i ++){
00085     for(j = i+1 ; j <= nAtom ; j ++){
00086       dr[1] = rx[i] - rx[j];
00087       if(fabs(dr[1]) > regionH[1])
00088     dr[1] -= SignR(region[1], dr[1]);
00089
00090      dr[2] = ry[i] - ry[j];
00091       if(fabs(dr[2]) > regionH[2])
00092     dr[2] -= SignR(region[2], dr[2]);
00093
00094      rr = Sqr(dr[1]) + Sqr(dr[2]);
```

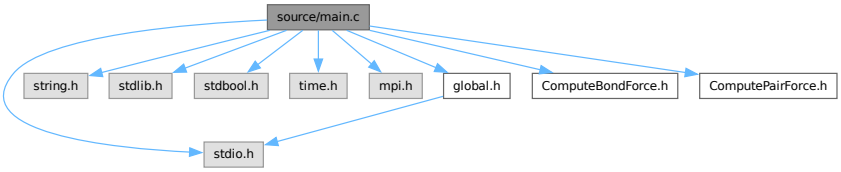
```
00095       if(rr < rrCut ){
00096       r = sqrt(rr);
00097       ri = 1/r;
00098       uVal = ri*exp(-kappa*r);
00099
00100       TVal = (1./rr + Sqr(kappa) + kappa/r)*uVal;
00101       TValSum[i] += TVal;
00102       TValSum[j] += TVal;
00103     } }
00104       AA = Sqr(ax[i]) + Sqr(ay[i]);
00105       AASum += AA;
00106       vv = Sqr(vx[i]) + Sqr(vy[i]);
00107       VVSum += vv;
00108       deno += TValSum[i];
00109 }
00110
00111       double gSumconfig, varSconfig, massSconfig;
00112       if(stepCount == 1) varSconfig = 0.;
00113       gSumconfig = 0.; massSconfig = 2.0;
00114
00115       gSumconfig = (AASum/temperature - deno)/massSconfig;
00116       varSconfig += deltaT*gSumconfig;
00117
00118        /*****Configarational Nose-Hoover thermostat*****/
00119     for (n = 1; n <= nAtom; n++){
00120        vx[n] += deltaT * ax[n];
00121        rx[n] += deltaT * (vx[n] + varSconfig * ax[n]);
00122        vy[n] += deltaT * ay[n];
00123        ry[n] += deltaT * (vy[n] + varSconfig * ay[n]);
00124      }
00125        /*****Kinetic Nose-Hoover thermostat*****/
00126    }else if(thermo == 'N'){
00127      gSum = (0.5*S2 - (nAtom + 1)*temperature)/massS;
00128      varS += deltaT*gSum;
00129     for (n = 1; n <= nAtom; n++){
00130        vx[n] += deltaT * (ax[n] - varS *vx[n]);
00131        rx[n] += deltaT * vx[n];
00132        vy[n] += deltaT * (ay[n] - varS *vy[n]);
00133        ry[n] += deltaT * vy[n];
00134     }
00135        /*****for Gaussian thermostat*****/
00136   }else if(thermo == 'G'){
00137        for (n = 1; n <= nAtom; n++){
00138        vx[n] = C * vx[n] + D * ax[n];
00139        rx[n] += deltaT * vx[n];
00140        vy[n] = C * vy[n] + D * ay[n];
00141        ry[n] += deltaT * vy[n];
00142       }
00143     }else if (thermo == 'L'){
00144    double nu = 0.03066;
00145    double var = sqrt(2*nu/(GAMMA*deltaT));
00146    double scale = 1. + nu*deltaT/2.;
00147    double scale_v = 2./scale - 1.;
00148    double scale_f = deltaT/scale;
00149    int n;
00150    for(n = 1 ; n <= nAtom ; n ++){
00151        vx[n] = scale_v*vx[n] + scale_f*(ax[n] + var*gsl_ran_gaussian(rnd,1));
00152        rx[n] += deltaT * vx[n];
00153        vy[n] = scale_v*vy[n] + scale_f*(ay[n] + var*gsl_ran_gaussian(rnd,1));
00154        ry[n] += deltaT * vy[n];
00155      }
00156    }
00157   }else{
00158      int n;
00159      for(n = 1 ; n <= nAtom ; n ++){
00160        vx[n] += deltaT * ax[n];
00161        rx[n] += deltaT * vx[n];
00162        vy[n] += deltaT * ay[n];
00163        ry[n] += deltaT * vy[n];
00164      }
00165    }
00166 }
00167
```

3.72 source/main.c File Reference

```
#include <stdio.h>
#include <string.h>
#include <stdlib.h>
#include <stdbool.h>
```

```
#include <time.h>
#include <mpi.h>
#include "global.h"
#include "ComputeBondForce.h"
#include "ComputePairForce.h"
```

Include dependency graph for main.c:



Macros

- #define DEFINE_GLOBALS

Functions

- void Init ()
- void SetupJob ()
- void EvalSpacetimeCorr ()
- void Trajectory ()
- void DumpState ()
- void ComputeForcesCells ()
- void LeapfrogStep ()
- void BrownianStep ()
- void ApplyBoundaryCond ()
- void EvalProps ()
- void EvalVacf ()
- void EvalRdf ()
- void AccumProps (int icode)
- void PrintSummary ()
- void PrintVrms ()
- void DumpBonds ()
- void VelocityVerletStep (int icode)
- void ApplyForce ()
- void ApplyDrivingForce ()
- void ApplyShear ()
- void ApplyLeesEdwardsBoundaryCond ()
- void PrintStress ()
- void Close ()
- void PrintMomentum ()
- void DisplaceAtoms ()
- void DumpRestart ()
- bool HaltConditionCheck (double value, int stepCount)
- void EvalCom ()
- void PrintCom ()
- void EvalVrms ()
- void EvalUnwrap ()
- void DumpPairs ()
- void ApplyViscous ()
- int main (int argc, char **argv)

Variables

- char * prefix = NULL

3.72.1 Macro Definition Documentation

3.72.1.1 DEFINE_GLOBALS

```
#define DEFINE_GLOBALS
```

Definition at line 7 of file main.c.

3.72.2 Function Documentation

3.72.2.1 AccumProps()

```
void AccumProps (
            int icode )
```

Definition at line 25 of file AccumProps.c.

```
00025                           {
00026   if(icode == 0){
00027   sPotEnergy = ssPotEnergy = 0.;
00028   sKinEnergy = ssKinEnergy = 0.;
00029   sPressure = ssPressure = 0.;
00030   sTotEnergy = ssTotEnergy = 0.;
00031   svirSum = 0.;
00032   }else if(icode == 1){
00033   sPotEnergy += potEnergy;
00034   ssPotEnergy += Sqr(potEnergy);
00035   sKinEnergy += kinEnergy;
00036   ssKinEnergy += Sqr(kinEnergy);
00037   sTotEnergy += totEnergy;
00038   ssTotEnergy += Sqr(totEnergy);
00039   sPressure += pressure;
00040   ssPressure += Sqr(pressure);
00041   svirSum += virSum;
00042   }else if(icode == 2){
00043   sPotEnergy /= stepAvg;
00044   ssPotEnergy /= sqrt(ssPotEnergy/stepAvg - Sqr(sPotEnergy));
00045   sTotEnergy /= stepAvg;
00046   ssTotEnergy = sqrt(ssTotEnergy/stepAvg - Sqr(sTotEnergy));
00047   sKinEnergy /= stepAvg;
00048   ssKinEnergy = sqrt(ssKinEnergy/stepAvg - Sqr(sKinEnergy));
00049   sPressure /= stepAvg;
00050   ssPressure = sqrt(ssPressure/stepAvg - Sqr(sPressure));
00051   svirSum /= stepAvg;
00052   } }
```

3.72.2.2 ApplyBoundaryCond()

```
void ApplyBoundaryCond ( )
```

Definition at line 27 of file ApplyBoundaryCond.c.

```
00027                           {
00028    int n;
00029    for(n = 1 ; n <= nAtom ; n ++){
00030     if(strcmp(xBoundary, "p") == 0 && strcmp(yBoundary, "p") == 0){         // P.B.C along x and y axis
00031      rx[n] -= region[1]*rint(rx[n]/region[1]);
00032      ry[n] -= region[2]*rint(ry[n]/region[2]);
00033     } else if (strcmp(xBoundary, "r") == 0 && strcmp(yBoundary, "r") == 0){    //R.B.C. along x and y
    axis
00034       if((rx[n] + atomRadius[n]) >= regionH[1]){
00035          rx[n] = 0.999999*regionH[1] - atomRadius[n]; vx[n] = -vx[n] ;
00036       }if((rx[n]-atomRadius[n]) < -regionH[1]){
```

```
00037         rx[n] = -0.999999*regionH[1] + atomRadius[n]; vx[n] = -vx[n] ;
00038      }
00039       if((ry[n] + atomRadius[n])>= regionH[2]){
00040          ry[n] = 0.999999*regionH[2] - atomRadius[n]; vy[n] = -vy[n] ;
00041       }if((ry[n]-atomRadius[n]) < -regionH[2]){
00042          ry[n] = -0.999999*regionH[2] + atomRadius[n]; vy[n] = -vy[n] ;
00043      }}
00044      else if (strcmp(xBoundary, "p") == 0 && strcmp(yBoundary, "r") == 0){   //P.B.C. along x and R.B.C
     along y axis
00045      rx[n] -= region[1]*rint(rx[n]/region[1]);
00046      if((ry[n] + atomRadius[n]) >= regionH[2]){
00047        ry[n] = 0.999999*regionH[2] - atomRadius[n]; vy[n] = -vy[n] ;
00048       }if((ry[n] - atomRadius[n]) < -regionH[2]){
00049          ry[n] = -0.999999*regionH[2] + atomRadius[n]; vy[n] = -vy[n] ;
00050    }}
00051      else if(strcmp(xBoundary, "r") == 0 && strcmp(yBoundary, "p") == 0){   //R.B.C. along x and P.B.C
     along y axis
00052      if((rx[n] + atomRadius[n]) >= regionH[1]){
00053         rx[n] = 0.999999*regionH[1] - atomRadius[n]; vx[n] = -vx[n] ;
00054       }if((rx[n] - atomRadius[n]) < -regionH[1]){
00055        rx[n] = -0.999999*regionH[1] + atomRadius[n]; vx[n] = -vx[n] ;
00056       }
00057       ry[n] -= region[2]*rint(ry[n]/region[2]);
00058    } else {
00059      // Print error message and exit the program
00060      fprintf(fpresult, "Error: Invalid boundary configuration: '%s %s'\n", xBoundary, yBoundary);
00061      exit(EXIT_FAILURE); // Exit with failure status
00062    }
00063   }
00064 }
```

References atomRadius, fpresult, nAtom, region, regionH, rx, ry, vx, vy, xBoundary, and yBoundary.

Referenced by main().

Here is the caller graph for this function:

3.72.2.3 ApplyDrivingForce()

```
void ApplyDrivingForce ( )
```

Definition at line 25 of file ApplyDrivingForce.c.

```
00025                          {
00026   int n;
00027   double Vxblock, Vyblock;
00028   double Vxsubstrate, Vysubstrate;
00029   Vxblock = 0.0;  Vyblock = 0.0;
00030   Vxsubstrate = 0.0; Vysubstrate = 0.0;
00031   double gammav;
00032   gammav = 0.0;
00033
00034   double count_substrate = 0;
00035   double count_block = 0;
00036
00037   for(n = 1 ; n <= nAtom; n ++){
00038    if(atomType[n] == 1 || atomType[n] == 2){
00039    Vxsubstrate += vx[n]; Vysubstrate += vy[n];
00040    count_substrate++;
00041    }
00042    if(atomType[n] == 3 || atomType[n] == 4){
00043    Vxblock += vx[n]; Vyblock += vy[n];
00044    count_block++;
```

```
00045   } }
00046
00047   if(count_substrate > 0) {
00048     Vxsubstrate /= count_substrate;
00049     Vysubstrate /= count_substrate;
00050   }
00051
00052   if(count_block > 0) {
00053    Vxblock /= count_block;
00054    Vyblock /= count_block;
00055   }
00056
00057  for(n = 1 ; n <= nAtom; n ++){
00058   if(atomType[n] == 1 || atomType[n] == 2){
00059   ax[n] += -gammav * (vx[n] - Vxsubstrate);
00060   ay[n] += -gammav * (vy[n] - Vysubstrate);
00061   }
00062   if(atomType[n] == 3 || atomType[n] == 4){
00063   ax[n] += -gammav * (vx[n] - Vxblock);
00064   ay[n] += -gammav * (vy[n] - Vyblock);
00065  } } }
```

References atomType, ax, ay, nAtom, vx, and vy.

3.72.2.4 ApplyForce()

```
void ApplyForce ( )
```

Definition at line 25 of file ApplyForce.c.

```
00025                   {
00026  int n;
00027  double lx;
00028  lx = regionH[1];
00029  fy =  (FyBylx * lx)/nAtomBlock;
00030  fx =  fxByfy * fy;
00031  for(n = 1; n <= nAtom; n ++){
00032  if(molID[n] == 2){
00033   ax[n] += fx;
00034   ay[n] -= fy;
00035 } } }
```

References ax, ay, fx, fxByfy, fy, FyBylx, molID, nAtom, nAtomBlock, and regionH.

Referenced by main().

Here is the caller graph for this function:

3.72.2.5 ApplyLeesEdwardsBoundaryCond()

```
void ApplyLeesEdwardsBoundaryCond ( )
```

Definition at line 25 of file ApplyLeesEdwardsBoundaryCond.c.

```
00025                                   {
00026  int n;
00027  for (n = 1; n <= nAtom; n++) {
```

```
00028 //PBC along x-direction
00029  if(rx[n] >= regionH[1])
00030    rx[n] -= region[1];
00031  else if(rx[n] < -regionH[1])
00032    rx[n] += region[1];
00033
00034 //LEBC along y-direction
00035   if(ry[n] >= regionH[2]){
00036    rx[n] -= shearDisplacement;
00037    if(rx[n] < -regionH[1]) rx[n] += region[1];
00038    //vx[n] -= shearVelocity;
00039    ry[n] -= region[2];
00040   }else if(ry[n] < -regionH[2]){
00041    rx[n] += shearDisplacement;
00042    if(rx[n] >= regionH[1]) rx[n] -= region[1];
00043    //vx[n] += shearVelocity;
00044    ry[n] += region[2];
00045   }
00046  }
00047 }
```

References nAtom, region, regionH, rx, ry, and shearDisplacement.

3.72.2.6 ApplyShear()

```
void ApplyShear ( )
```

Definition at line 25 of file ApplyShear.c.

```
00025                  {
00026  int n;
00027  for(n = 1 ; n <= nAtom ; n ++){
00028   rx[n] += strain * ry[n];
00029   //vx[n] += stranRate * ry[n];
00030  } }
```

References nAtom, rx, ry, and strain.

3.72.2.7 ApplyViscous()

```
void ApplyViscous ( )
```

Definition at line 25 of file ApplyViscous.c.

```
00025                    {
00026  int n;
00027  double gammav;
00028  gammav = 1.0;
00029  for(n = 1 ; n <= nAtom; n ++){
00030   ax[n] += -gammav * vx[n];
00031   ay[n] += -gammav * vy[n];
00032  } }
```

References ax, ay, nAtom, vx, and vy.

3.72.2.8 BrownianStep()

```
void BrownianStep ( )
```

Definition at line 26 of file BrownianStep.c.

```
00026                    {
00027   if(stepCount <= stepEquil){
00028     double A, S1, S2, T;
00029     int n;
00030     S1 = 0.; S2 = 0;
00031     double halfdt = 0.5*deltaT;
00032     for (n = 1; n <= nAtom; n++){
00033       T = vx[n] + halfdt * ax[n];
00034       S1 += T * ax[n];
00035       S2 += Sqr(T);
```

```
00036
00037       T = vy[n] + halfdt * ay[n];
00038       S1 += T * ay[n];
00039       S2 += Sqr(T);
00040     }
00041     A = -S1 / S2;
00042     double C = 1 + A*deltaT ;
00043     double D = deltaT * (1 + 0.5 * A * deltaT);
00044     for (n = 1; n <= nAtom; n++){
00045       vx[n] = C * vx[n] + D * ax[n];
00046       rx[n] += deltaT * vx[n];
00047       vy[n] = C * vy[n] + D * ay[n];
00048       ry[n] += deltaT * vy[n];
00049     }
00050   }else{
00051       int n;
00052       //SETTING TEMP = 0.0
00053      if (stepCount == stepEquil+1){
00054      for(n = 1 ; n <= nAtom ; n ++){
00055      vx[n] = 0.0;
00056      vy[n] = 0.0;
00057      }}
00058      double zeta = 1.0;
00059      double dx, dy;
00060      for(n = 1 ; n <= nAtom ; n ++){
00061       dx = rx[n];
00062       rx[n] += zeta * ax[n] * deltaT;
00063       dx = rx[n] - dx;
00064       vx[n] = dx/deltaT;
00065       dy = ry[n];
00066       ry[n] += zeta * ay[n] * deltaT;
00067       dy = ry[n] - dy;
00068       vy[n] = dy/deltaT;
00069     }
00070   }
00071 }
```

References ax, ay, deltaT, nAtom, rx, ry, Sqr, stepCount, stepEquil, vx, and vy.

3.72.2.9 Close()

```
void Close ( )
```

Definition at line 24 of file Close.c.

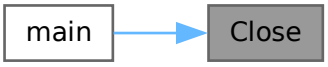
```
00024            {
00025   int n;
00026   free(rx);
00027   free(ry);
00028   free(vx);
00029   free(vy);
00030   free(ax);
00031   free(ay);
00032   free(fax);
00033   free(fay);
00034   free(cellList);
00035
00036   free(atomID); free(atomType); free(atomRadius); free(atomMass);
00037   free(speed);
00038   free(atom1); free(atom2); free(BondID);
00039   free(BondType); free(kb); free(ro);
00040   free(ImageX); free(ImageY); free(rxUnwrap); free(ryUnwrap);
00041   free(atomIDInterface);
00042   free(PairID); free(Pairatom1); free(Pairatom2);
00043   free(PairXij); free(PairYij);
00044
00045   free(DeltaXijOld);
00046   free(DeltaYijOld);
00047
00048   free(molID);
00049
00050   for (n = 0; n <= nAtom; n++) {
00051    free(isBonded[n]);
00052    }
00053    free(isBonded);
00054
00055
00056
00057   for(n = 0; n <= nAtom; n++) {
00058    free(DeltaXijOldPair[n]);
00059    free(DeltaYijOldPair[n]);
00060    }
```

```
00061     free(DeltaXijOldPair);
00062     free(DeltaYijOldPair);
00063
00064   for (n = 0; n <= nBuffCorr; n++){
00065     free(cfOrg[n]);
00066     free(spacetimeCorr[n]);
00067   }
00068   free(cfOrg);
00069   free(spacetimeCorr);
00070   free(cfVal);
00071   free(indexCorr);
00072   free(spacetimeCorrAv);
00073
00074   free(indexAcf);
00075   free(viscAcfOrg);
00076   free(viscAcfAv);
00077   for(n = 0 ; n <= nBuffAcf ; n ++)
00078     free(viscAcf[n]);
00079   free(viscAcf);
00080
00081 }
```

References atom1, atom2, atomID, atomIDInterface, atomMass, atomRadius, atomType, ax, ay, BondID, BondType, cellList, cfOrg, cfVal, DeltaXijOld, DeltaXijOldPair, DeltaYijOld, DeltaYijOldPair, fax, fay, ImageX, ImageY, indexAcf, indexCorr, isBonded, kb, molID, nAtom, nBuffAcf, nBuffCorr, Pairatom1, Pairatom2, PairID, PairXij, PairYij, ro, rx, rxUnwrap, ry, ryUnwrap, spacetimeCorr, spacetimeCorrAv, speed, viscAcf, viscAcfAv, viscAcfOrg, vx, and vy.

Referenced by main().

Here is the caller graph for this function:



3.72.2.10 ComputeForcesCells()

```
void ComputeForcesCells ( )
```

Definition at line 25 of file ComputeForcesCells.c.

```
00025                           {
00026   double dr[NDIM+1], invWid[NDIM+1], shift[NDIM+1], f, fcVal, rr, ri, r, uVal;
00027   int c, I, J, m1, m1X, m1Y, m2, m2X, m2Y, n, offset;
00028   int iofX[] = {0, 0, 1, 1, 0, -1, -1, -1, 0, 1},
00029       iofY[] = {0, 0, 0, 1 ,1, 1, 0, -1, -1, -1};
00030
00031   invWid[1] = cells[1]/region[1];
00032   invWid[2] = cells[2]/region[2];
00033
00034   for(n = nAtom+1; n <= nAtom+cells[1]*cells[2] ; n++)
00035     cellList[n] = 0;
00036
00037   for(n = 1 ; n <= nAtom ; n ++){
00038     c = ((int)((ry[n] + regionH[2])*invWid[2]))*cells[1] + (int)((rx[n]+regionH[1])*invWid[1]) +
      nAtom+ 1;
00039     cellList[n] = cellList[c];
00040     cellList[c] = n;
00041   }
00042
00043   for(n = 1 ; n <= nAtom ; n ++){
00044     ax[n] = 0.;
00045     ay[n] = 0.;
00046   }
```

```
00047
00048   uSum = 0.0 ;
00049   virSum = 0.0;
00050   rfAtom = 0.0;
00051   RadiusIJ = 0.0;
00052
00053   gamman = 1.0;
00054   double vr[NDIM+1], fd, fdVal, rrinv;
00055   rrinv = 0.0;
00056   fd = 0.0;
00057   fdVal = 0.0;
00058
00059   int start = 1 + rank*(cells[2]/size);
00060   int end = (rank+1)*(cells[2]/size);
00061
00062   for(m1Y = start ; m1Y <= end ; m1Y ++){
00063     for(m1X = 1 ; m1X <= cells[1] ; m1X ++){
00064       m1 = (m1Y-1) * cells[1] + m1X + nAtom;
00065       for(offset = 1 ; offset <= 9 ; offset ++){
00066     m2X = m1X + iofX[offset]; shift[1] = 0.;
00067     if(m2X > cells[1]){
00068       m2X = 1; shift[1] = region[1];
00069     }else if(m2X == 0){
00070       m2X = cells[1]; shift[1] = -region[1];
00071     }
00072     m2Y = m1Y + iofY[offset]; shift[2] = 0.;
00073     if(m2Y > cells[2]){
00074       m2Y = 1; shift[2] = region[2];
00075     }else if(m2Y == 0){
00076       m2Y = cells[2]; shift[2] = -region[2];
00077     }
00078     m2 = (m2Y-1)*cells[1] + m2X + nAtom;
00079     I = cellList[m1];
00080     while(I > 0){
00081       J = cellList[m2];
00082       while(J > 0){
00083         if(m1 == m2 && J != I && (atomRadius[I] > 0. && atomRadius[J] > 0.)){
00084           dr[1] = rx[I] - rx[J] - shift[1];
00085           dr[2] = ry[I] - ry[J] - shift[2];
00086           rr = Sqr(dr[1]) + Sqr(dr[2]);
00087           RadiusIJ = atomRadius[I] + atomRadius[J];
00088           SqrRadiusIJ = Sqr(RadiusIJ);
00089           if(rr < SqrRadiusIJ){
00090         r = sqrt(rr);
00091         ri = 1.0/r;
00092                 rrinv = 1.0/rr;
00093                 vr[1] = vx[I] - vx[J];
00094                 vr[2] = vy[I] - vy[J];
00095         RadiusIJInv = 1.0/RadiusIJ;
00096         uVal = Sqr(1.0 - r * RadiusIJInv);
00097         fcVal = 2.0 * RadiusIJInv * (1.0 - r * RadiusIJInv) *ri;
00098                 fdVal = -gamman * (vr[1]*dr[1] + vr[2]*dr[2]) * rrinv; //disc-disc drag
00099
00100         f  = fcVal * dr[1];
00101                 fd = fdVal * dr[1];
00102         ax[I] += (f + fd);
00103                 discDragx[I] += fd; //disc-disc drag
00104
00105         f = fcVal * dr[2];
00106                 fd = fdVal * dr[2];
00107         ay[I] += (f + fd);
00108                 discDragy[I] += fd; //disc-disc drag
00109
00110         uSum +=  0.5 * uVal;
00111         virSum += 0.5 * fcVal * rr;
00112         rfAtom += 0.5 * dr[1] * fcVal * dr[2];
00113           }
00114         }else if(m1 != m2 && (atomRadius[I] > 0. && atomRadius[J] > 0.)){
00115           dr[1] = rx[I] - rx[J] - shift[1];
00116           dr[2] = ry[I] - ry[J] - shift[2];
00117           rr = Sqr(dr[1]) + Sqr(dr[2]);
00118           RadiusIJ = atomRadius[I] + atomRadius[J];
00119           SqrRadiusIJ = Sqr(RadiusIJ);
00120           if(rr < SqrRadiusIJ){
00121         r = sqrt(rr);
00122         ri = 1.0/r;
00123                 rrinv = 1.0/r;
00124                 vr[1] = vx[I] - vx[J];
00125                 vr[2] = vy[I] - vy[J];
00126         RadiusIJInv = 1.0/RadiusIJ;
00127         uVal = Sqr(1.0 - r * RadiusIJInv);
00128         fcVal = 2.0 * RadiusIJInv * (1.0 - r * RadiusIJInv) *ri;
00129                 fdVal = -gamman * (vr[1]*dr[1] + vr[2]*dr[2]) * rrinv; //disc-disc drag
00130
00131         f  = fcVal * dr[1];
00132                 fd =  fdVal * dr[1];
00133         ax[I] += (f + fd);
```

```
00134                 discDragx[I] += fd; //disc-disc drag
00135
00136         f   = fcVal * dr[2];
00137                 fd = fdVal * dr[2];
00138         ay[I] += (f + fd);
00139                 discDragy[I] += fd; //disc-disc drag
00140
00141         uSum +=  0.5 * uVal;
00142         virSum += 0.5 * fcVal * rr;
00143         rfAtom += 0.5 * dr[1] * fcVal * dr[2];
00144           }
00145         }
00146             J = cellList[J];
00147       }
00148       I = cellList[I];
00149     }
00150       }
00151     }
00152   }
00153 }
```

References atomRadius, ax, ay, cellList, cells, discDragx, discDragy, gamman, nAtom, NDIM, RadiusIJ, RadiusIJInv, rank, region, regionH, rfAtom, rx, ry, size, Sqr, SqrRadiusIJ, uSum, virSum, vx, and vy.

3.72.2.11 DisplaceAtoms()

```
void DisplaceAtoms ( )
```

Definition at line 25 of file DisplaceAtoms.c.

```
00025                     {
00026  int n;
00027   for(n = 1; n <= nAtom; n ++){
00028    if(molID[n] == 2){
00029     rx[n] += DeltaX;
00030     ry[n] += DeltaY;
00031 } } }
```

References DeltaX, DeltaY, molID, nAtom, rx, and ry.

Referenced by main().

Here is the caller graph for this function:

3.72.2.12 DumpBonds()

```
void DumpBonds ( )
```

Definition at line 24 of file DumpBonds.c.

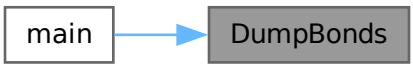
```
00024                 {
00025   int n;
00026   //Trajectory file in LAMMPS dump format for OVITO visualization
00027   fprintf(fpbond, "ITEM: TIMESTEP\n");
00028   fprintf(fpbond, "%lf\n",timeNow);
00029   fprintf(fpbond, "ITEM: NUMBER OF ENTRIES\n");
00030   fprintf(fpbond, "%d\n",nBond);
```

```
00031   fprintf(fpbond, "ITEM: BOX BOUNDS pp ff pp\n");
00032   fprintf(fpbond, "%lf %lf xlo xhi\n", -regionH[1], regionH[1]);
00033   fprintf(fpbond, "%lf %lf ylo yhi\n", -regionH[2], regionH[2]);
00034   fprintf(fpbond, "%lf %lf zlo zhi\n", -0.1, 0.1);
00035   fprintf(fpbond, "ITEM: ENTRIES BondID, BondType, atom1 atom2 BondLength BondLengthEqul nodeDragx1
      nodeDragy1\n");
00036
00037   for(n=1; n<=nBond; n++)
00038    fprintf(fpbond, "%d %d %d %d %0.16lf %0.16lf %0.16lf %0.16lf\n", BondID[n], BondType[n], atom1[n],
      atom2[n],
00039    BondLength[n], ro[n], nodeDragx[atom1[n]], nodeDragy[atom1[n]]);
00040   }
```

References atom1, atom2, BondID, BondLength, BondType, fpbond, nBond, nodeDragx, nodeDragy, regionH, ro, and timeNow.

Referenced by main().

Here is the caller graph for this function:



3.72.2.13 DumpPairs()

```
void DumpPairs ( )
```

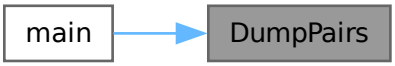
Definition at line 25 of file DumpPairs.c.

```
00025                {
00026   int n;
00027   //Trajectory file in LAMMPS dump format for OVITO visualization
00028   fprintf(fppair, "ITEM: TIMESTEP\n");
00029   fprintf(fppair, "%lf\n",timeNow);
00030   fprintf(fppair, "ITEM: NUMBER OF ENTRIES\n");
00031   fprintf(fppair, "%d\n",nPairActive);
00032   fprintf(fppair, "ITEM: BOX BOUNDS pp ff pp\n");
00033   fprintf(fppair, "%lf %lf xlo xhi\n", -regionH[1], regionH[1]);
00034   fprintf(fppair, "%lf %lf ylo yhi\n", -regionH[2], regionH[2]);
00035   fprintf(fppair, "%lf %lf zlo zhi\n", -0.1, 0.1);
00036   fprintf(fppair, "ITEM: ENTRIES index, atom1 atom2 xij yij discDragx1 discDragy1\n");
00037
00038   for(n=1; n<=nPairActive; n++)
00039    fprintf(fppair, "%d %d %d %0.16lf %0.16lf %0.16lf %0.16lf\n", PairID[n], Pairatom1[n],
      Pairatom2[n],
00040    PairXij[n], PairYij[n], discDragx[n], discDragy[n]);
00041
00042   }
```

References discDragx, discDragy, fppair, nPairActive, Pairatom1, Pairatom2, PairID, PairXij, PairYij, regionH, and timeNow.

Referenced by main().

Here is the caller graph for this function:



3.72.2.14 DumpRestart()

```
void DumpRestart ( )
```

Definition at line 25 of file DumpRestart.c.

```
00025                     {
00026  char DUMP[256];
00027  FILE *fpDUMP;
00028  sprintf(DUMP, "%s.Restart", prefix);
00029  fpDUMP = fopen(DUMP, "w");
00030  if(fpDUMP == NULL) {
00031   fprintf(stderr, "Error opening file %s for writing\n", DUMP);
00032   return;
00033  }
00034
00035   fprintf(fpDUMP, "timeNow %lf\n", timeNow);
00036   fprintf(fpDUMP, "nAtom %d\n",  nAtom);
00037   fprintf(fpDUMP, "nBond %d\n", nBond);
00038   fprintf(fpDUMP, "nAtomType %d\n", nAtomType);
00039   fprintf(fpDUMP, "nBondType %d\n", nBondType);
00040   fprintf(fpDUMP, "region[1] %0.14lf\n", region[1]);
00041   fprintf(fpDUMP, "region[2] %0.14lf\n", region[2]);
00042
00043   int n;
00044   fprintf(fpDUMP, "Atoms\n");
00045   for(n = 1; n <= nAtom; n ++)
00046    fprintf(fpDUMP, "%d %d %d %0.2lf %0.16lf %0.16lf %0.16lf %0.16lf\n", atomID[n], molID[n],
      atomType[n], atomRadius[n], rx[n], ry[n], vx[n], vy[n]);
00047
00048
00049   fprintf(fpDUMP, "Bonds\n");
00050   for(n=1; n<=nBond; n++)
00051   fprintf(fpDUMP,  "%d %d %d %d %0.2lf %0.16lf\n", BondID[n], BondType[n], atom1[n], atom2[n], kb[n],
      ro[n]);
00052
00053   fclose(fpDUMP);
00054 }
```

References atom1, atom2, atomID, atomRadius, atomType, BondID, BondType, kb, molID, nAtom, nAtomType, nBond, nBondType, prefix, region, ro, rx, ry, timeNow, vx, and vy.

Referenced by main().

Here is the caller graph for this function:

3.72.2.15 DumpState()

```
void DumpState ( )
```

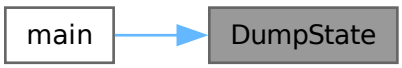
Definition at line 25 of file DumpState.c.

```
00025                  {
00026  char DUMP[256];
00027  FILE *fpDUMP;
00028  sprintf(DUMP, "%s.STATE", prefix);
00029  fpDUMP = fopen(DUMP, "w");
00030  if(fpDUMP == NULL) {
00031   fprintf(stderr, "Error opening file %s for writing\n", DUMP);
00032   return;
00033  }
00034
00035   fprintf(fpDUMP, "ITEM: TIMESTEP\n");
00036   fprintf(fpDUMP, "%lf\n",timeNow);
00037   fprintf(fpDUMP, "ITEM: NUMBER OF ATOMS\n");
00038   fprintf(fpDUMP, "%d\n",nAtom);
00039   fprintf(fpDUMP, "ITEM: BOX BOUNDS pp pp pp\n");
00040   fprintf(fpDUMP, "%lf %lf xlo xhi\n", -regionH[1], regionH[1]);
00041   fprintf(fpDUMP, "%lf %lf ylo yhi\n", -regionH[2], regionH[2]);
00042   fprintf(fpDUMP, "%lf %lf zlo zhi\n",  -0.1, 0.1);
00043   fprintf(fpDUMP, "ITEM: ATOMS id mol type radius x y vx vy fx fy\n");
00044   int n;
00045   for (n = 1; n <= nAtom; n++) {
00046    fprintf(fpDUMP, "%d\t %d\t %d\t %0.2lf\t %0.16lf\t %0.16lf\t %0.16lf\t %0.16lf\t %0.16lf\t
      %0.16lf\n",
00047    atomID[n], molID[n], atomType[n], atomRadius[n], rx[n], ry[n], vx[n], vy[n], ax[n], ay[n]);
00048   }
00049   fclose(fpDUMP);
00050 }
```

References atomID, atomRadius, atomType, ax, ay, molID, nAtom, prefix, regionH, rx, ry, timeNow, vx, and vy.

Referenced by main().

Here is the caller graph for this function:



3.72.2.16 EvalCom()

```
void EvalCom ( )
```

Definition at line 27 of file EvalCom.c.

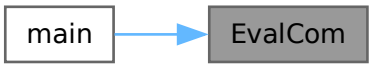
```
00027                 {
00028  int n;
00029  ComX = 0.0; ComY = 0.0; ComXRatio = 0.0; ComYRatio = 0.0;
00030  TotalMass = 0.0;
00031
00032  for(n=1; n<=nAtom; n++){
00033  if(molID[n] == 2){
00034   ComX += atomMass[n] * rxUnwrap[n];
00035   ComY += atomMass[n] * ryUnwrap[n];
00036   TotalMass += atomMass[n];
00037   } }
00038
00039   ComX = ComX/TotalMass;
00040   ComY = ComY/TotalMass;
00041
```

```
00042   if(timeNow == 0.0){
00043   ComX0 = ComX; ComY0 = ComY;
00044   }
00045   ComXRatio = ComX/ComX0;   ComYRatio = ComY/ComY0;
00046  }
```

References atomMass, ComX, ComX0, ComXRatio, ComY, ComY0, ComYRatio, molID, nAtom, rxUnwrap, ryUnwrap, timeNow, and TotalMass.

Referenced by main().

Here is the caller graph for this function:



3.72.2.17 EvalProps()

```
void EvalProps ( )
```

Definition at line 26 of file EvalProps.c.

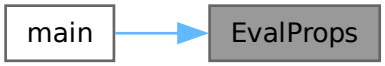
```
00026                   {
00027  real v, vv;
00028  virSum = 0.0;
00029  vSumX = 0.0; vSumY = 0.0; vSum = 0.0;
00030  vvSum = 0.;
00031  int n;
00032
00033  for (n = 1; n <= nAtom; n++) {
00034   vv = 0.;
00035   // Initialize v with a default value to avoid "uninitialized" warning.
00036   v = 0.0;
00037   // X direction velocity
00038   if (strcmp(solver, "Verlet") == 0) {
00039     v = vx[n];
00040   } else if (strcmp(solver, "LeapFrog") == 0) {
00041     v = vx[n] - 0.5 * deltaT * ax[n];
00042   }
00043    vSum += v;
00044    vv += Sqr(v);
00045    vSumX += v;
00046    // Y direction velocity
00047    if (strcmp(solver, "Verlet") == 0) {
00048    v = vy[n];
00049    } else if (strcmp(solver, "LeapFrog") == 0) {
00050    v = vy[n] - 0.5 * deltaT * ay[n];
00051    }
00052    vSum += v;
00053    vSumY += v;
00054    vv += Sqr(v);
00055    vvSum += vv;
00056   }
00057
00058   kinEnergy = 0.5 * vvSum / nAtom ;
00059   uSumPairPerAtom = uSumPair / nAtom ;
00060   BondEnergyPerAtom = TotalBondEnergy / (0.5*nAtom); //Factor of 0.5 since each atom has one half the
      bond energy
00061   potEnergy = uSumPairPerAtom +  BondEnergyPerAtom ;
00062   totEnergy = kinEnergy + potEnergy;
00063   virSumxx = virSumPairxx  + virSumBondxx ;
00064   virSumyy = virSumPairyy  + virSumBondyy ;
00065   virSumxy = virSumPairxy  + virSumBondxy ;
00066   virSum = virSumPair + virSumBond;
00067   pressure = density * (vvSum + virSum) / (nAtom * NDIM);
```

```
00068
00069 }
```

References ax, ay, BondEnergyPerAtom, deltaT, density, kinEnergy, nAtom, NDIM, potEnergy, pressure, solver, Sqr, TotalBondEnergy, totEnergy, uSumPair, uSumPairPerAtom, virSum, virSumBond, virSumBondxx, virSumBondxy, virSumBondyy, virSumPair, virSumPairxx, virSumPairxy, virSumPairyy, virSumxx, virSumxy, virSumyy, vSum, vSumX, vSumY, vvSum, vx, and vy.

Referenced by main().

Here is the caller graph for this function:



3.72.2.18 EvalRdf()

```
void EvalRdf ( )
```

Definition at line 26 of file EvalRdf.c.

```
00026                {
00027   real dr[NDIM+1], deltaR, normFac, rr, rrRange;
00028   int j1, j2, n;
00029   countRdf ++;
00030   if(countRdf == 1){
00031     for(n = 1 ; n <= sizeHistRdf ; n ++)
00032       histRdf[n] = 0.;
00033   }
00034   rrRange = Sqr(rangeRdf);
00035   deltaR = rangeRdf / sizeHistRdf;
00036   for(j1 = 1 ; j1 <= nAtom - 1 ; j1 ++){
00037     for(j2 = j1 + 1 ; j2 <= nAtom ; j2 ++){
00038
00039       dr[1] = rx[j1] - rx[j2];
00040       if(fabs(dr[1]) > regionH[1])
00041     dr[1] -= SignR(region[1], dr[1]);
00042
00043       dr[2] = ry[j1] - ry[j2];
00044       if(fabs(dr[2]) > regionH[2])
00045     dr[2] -= SignR(region[2], dr[2]);
00046
00047       rr = Sqr(dr[1]) + Sqr(dr[2]);
00048
00049       if(rr < rrRange){
00050     n = (int)(sqrt(rr)/deltaR) + 1;
00051     histRdf[n] ++;
00052       }
00053     }
00054   }
00055
00056   if(countRdf == limitRdf){
00057     normFac = region[1]*region[2] / (M_PI*Sqr(deltaR)*nAtom*nAtom*countRdf );
00058     for(n = 1 ; n <= sizeHistRdf ; n ++)
00059       histRdf[n] *= normFac/(n-0.5);
00060     // PRINT THE RADIAL DISTRIBUTION DATA ON TO DISK FILE
00061     real rBin;
00062     int n;
00063     fprintf(fprdf,"rdf @ timeNow %lf\n", timeNow);
00064     for(n = 1 ; n <= sizeHistRdf ; n ++){
00065       rBin = (n - 0.5)*rangeRdf/sizeHistRdf;
00066       fprintf(fprdf, "%lf %lf\n", rBin, histRdf[n]);
00067     }
00068   }
00069
00070 }
```

References countRdf, fprdf, histRdf, limitRdf, nAtom, NDIM, rangeRdf, region, regionH, rx, ry, SignR, sizeHistRdf, Sqr, and timeNow.

3.72.2.19 EvalSpacetimeCorr()

```
void EvalSpacetimeCorr ( )
```

Definition at line 26 of file EvalSpacetimeCorr.c.

```
00026                           {
00027   real cosV=0., cosV0=0., cosV1=0., cosV2=0., sinV=0., sinV1=0., sinV2=0.;
00028   real COSA, SINA, COSV, SINV;
00029   int j, m, n, nb, ni, nv;
00030   real kMin = 2. * M_PI / region[1];
00031   real kMax = M_PI;
00032   real deltaK = (kMax - kMin) / nFunCorr;
00033
00034   for (j = 1; j <= 2*nFunCorr; j++)
00035     cfVal[j] = 0.;
00036
00037   for (n = 1; n <= nAtom; n++){
00038     j = 1;
00039     COSA = cos(kMin*rx[n]);
00040     SINA = sin(kMin*rx[n]);
00041     for (m = 1; m <= nFunCorr; m++){
00042       if(m == 1){
00043     cosV = cos(deltaK*rx[n]);
00044     sinV = sin(deltaK*rx[n]);
00045     cosV0 = cosV;
00046       }else if(m == 2){
00047     cosV1 = cosV;
00048     sinV1 = sinV;
00049     cosV = 2.*cosV0*cosV1-1;
00050     sinV = 2.*cosV0*sinV1;
00051       }else{
00052     cosV2 = cosV1;
00053     sinV2 = sinV1;
00054     cosV1 = cosV;
00055     sinV1 = sinV;
00056     cosV = 2.*cosV0*cosV1-cosV2;
00057     sinV = 2.*cosV0*sinV1-sinV2;
00058       }
00059       COSV = COSA*cosV - SINA*sinV;
00060       SINV = SINA*cosV + COSA*sinV;
00061       cfVal[j] += COSV;
00062       cfVal[j+1] += SINV;
00063       j += 2;
00064     }
00065   }
00066
00067   for (nb = 1; nb <= nBuffCorr; nb++){
00068     indexCorr[nb] += 1;
00069     if (indexCorr[nb] <= 0) continue;
00070     ni = nFunCorr * (indexCorr[nb] - 1);
00071     if (indexCorr[nb] == 1){
00072       for (j = 1; j <= 2*nFunCorr; j++)
00073     cfOrg[nb][j] = cfVal[j];
00074     }
00075
00076     for (j = 1; j <= nFunCorr; j++)
00077       spacetimeCorr[nb][ni + j] = 0.;
00078
00079     j = 1;
00080     for (m = 1; m <= nFunCorr; m++){
00081       nv = m + ni;
00082       spacetimeCorr[nb][nv] += cfVal[j] * cfOrg[nb][j] + cfVal[j + 1] * cfOrg[nb][j + 1];
00083       j += 2;
00084     }
00085
00086   }
00087
00088   // ACCUMULATE SPACETIME CORRELATIONS
00089   for (nb = 1; nb <= nBuffCorr; nb++){
00090    if (indexCorr[nb] == nValCorr){
00091      for (j = 1; j <= nFunCorr*nValCorr; j++)
00092        spacetimeCorrAv[j] += spacetimeCorr[nb][j];
00093     indexCorr[nb] = 0.;
00094     countCorrAv ++;
00095     if (countCorrAv == limitCorrAv){
00096       for (j = 1; j <= nFunCorr*nValCorr; j++)
00097     spacetimeCorrAv[j] /= (nAtom*limitCorrAv);
00098       fprintf(fpdnsty,"NDIM %d\n", NDIM);
00099       fprintf(fpdnsty,"nAtom %d\n", nAtom);
00100       fprintf(fpdnsty,"region %lf\n", region[1]);
00101       fprintf(fpdnsty,"nFunCorr %d\n", nFunCorr);
00102       fprintf(fpdnsty,"limitCorrAv %d\n", limitCorrAv);
00103       fprintf(fpdnsty,"stepCorr %d\n", stepCorr);
00104       fprintf(fpdnsty,"nValCorr %d\n", nValCorr);
00105       fprintf(fpdnsty,"deltaT %lf\n", deltaT);
```

```
00106         real tVal;
00107         for (n = 1; n <= nValCorr; n++){
00108       tVal = (n-1)*stepCorr*deltaT;
00109       fprintf (fpdnsty, "%e\t", tVal);
00110       int nn = nFunCorr*(n-1);
00111       for (j = 1; j <= nFunCorr; j ++)
00112             fprintf (fpdnsty, "%e\t", spacetimeCorrAv[nn + j]);
00113           fprintf (fpdnsty, "\n");
00114         }
00115
00116         countCorrAv = 0.;
00117         for (j = 1; j <= nFunCorr*nValCorr; j++)
00118       spacetimeCorrAv[j] = 0.;
00119       }
00120     }
00121   }
00122 }
```

References cfOrg, cfVal, countCorrAv, deltaT, fpdnsty, indexCorr, limitCorrAv, nAtom, nBuffCorr, NDIM, nFunCorr, nValCorr, region, rx, spacetimeCorr, spacetimeCorrAv, and stepCorr.

3.72.2.20 EvalUnwrap()

```
void EvalUnwrap ( )
```

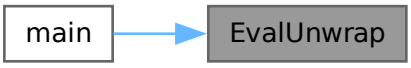
Definition at line 27 of file EvalUnwrap.c.

```
00027                   {
00028   int n;
00029   for (n = 1; n <= nAtom; n++) {
00030     rxUnwrap[n] = rx[n] + ImageX[n] * region[1];
00031     ryUnwrap[n] = ry[n] + ImageY[n] * region[2];
00032     }
00033 }
```

References ImageX, ImageY, nAtom, region, rx, rxUnwrap, ry, and ryUnwrap.

Referenced by main().

Here is the caller graph for this function:



3.72.2.21 EvalVacf()

```
void EvalVacf ( )
```

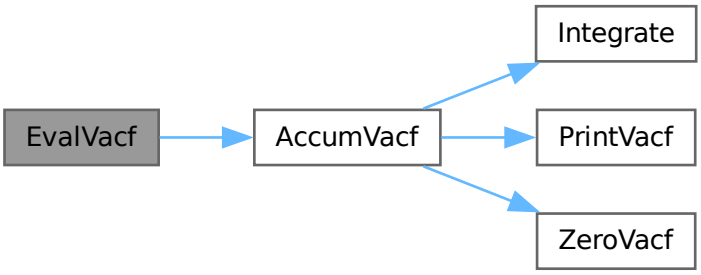
Definition at line 26 of file EvalVacf.c.

```
00026                 {
00027   int n, nb, ni;
00028   double viscVec = 0.;
00029   double v[3];
00030   for(n = 1 ; n <= nAtom ; n ++){
00031     v[1] = vx[n] - 0.5*ax[n]*deltaT;
00032     v[2] = vy[n] - 0.5*ay[n]*deltaT;
00033     viscVec += v[1]*v[2];
00034   }
00035   viscVec += rfAtom;
```

```
00036   for(nb = 1 ; nb <= nBuffAcf ; nb ++){
00037     indexAcf[nb] ++;
00038     if(indexAcf[nb] <= 0)continue;
00039     if(indexAcf[nb] == 1){
00040       viscAcfOrg[nb] = viscVec;
00041     }
00042     ni = indexAcf[nb];
00043     viscAcf[nb][ni] = viscAcfOrg[nb]*viscVec;
00044   }
00045   AccumVacf();
00046 }
```

References AccumVacf(), ax, ay, deltaT, indexAcf, nAtom, nBuffAcf, rfAtom, viscAcf, viscAcfOrg, vx, and vy.

Here is the call graph for this function:



3.72.2.22 EvalVrms()

```
void EvalVrms ( )
```

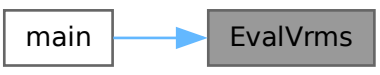
Definition at line 27 of file EvalVrms.c.

```
00027                {
00028   int n;
00029   VSqr = 0.0;
00030   VMeanSqr = 0.0;
00031   VRootMeanSqr = 0.0;
00032
00033   for(n = 1 ; n <= nAtom ; n ++){
00034   VSqr += Sqr(vx[n]) + Sqr(vy[n]);
00035   }
00036   VMeanSqr = VSqr/nAtom;
00037   VRootMeanSqr = sqrt(VMeanSqr);
00038   }
```

References nAtom, Sqr, VMeanSqr, VRootMeanSqr, VSqr, vx, and vy.

Referenced by main().

Here is the caller graph for this function:



3.72.2.23 HaltConditionCheck()

```
bool HaltConditionCheck (
            double value,
            int stepCount )
```

Definition at line 27 of file Halt.c.

```
00027                                                   {
00028
00029   if(value <= HaltCondition && value != 0) {
00030   fprintf(fpresult, "Halt condition met at step = %d with Vrms = %.10f\n", stepCount, value);
00031   return true;       // Signal that the halt condition is met
00032   }
00033  return false; // Halt condition not met
00034 }
```

References fpresult, HaltCondition, and stepCount.

Referenced by main().

Here is the caller graph for this function:

3.72.2.24 Init()

```
void Init ( )
```

Definition at line 29 of file Init.c.

```
00029           {
00030   char dummy[128];
00031   char inputConfig[128];
00032   FILE *fp;
00033   fp = fopen("input-data","r");
00034   fscanf(fp, "%s %s", dummy, inputConfig);
00035   fscanf(fp, "%s %s", dummy, solver);
00036   fscanf(fp, "%s %s %s", dummy, xBoundary, yBoundary);
00037   fscanf(fp, "%s %d",  dummy, &DampFlag);
00038   fscanf(fp, "%s %d",  dummy, &freezeAtomType);
00039   fscanf(fp, "%s %lf", dummy, &rCut);
00040   fscanf(fp, "%s %lf", dummy, &gamman);
00041   fscanf(fp, "%s %lf", dummy, &kappa);
00042   fscanf(fp, "%s %lf", dummy, &deltaT);
00043   fscanf(fp, "%s %lf", dummy, &strain);
00044   fscanf(fp, "%s %lf", dummy, &FyBylx);
00045   fscanf(fp, "%s %lf", dummy, &fxByfy);
00046   fscanf(fp, "%s %lf", dummy, &DeltaY);
00047   fscanf(fp, "%s %lf", dummy, &DeltaX);
00048   fscanf(fp, "%s %lf", dummy, &HaltCondition);
00049   fscanf(fp, "%s %d",  dummy, &stepAvg);
00050   fscanf(fp, "%s %d",  dummy, &stepEquil);
00051   fscanf(fp, "%s %d",  dummy, &stepLimit);
00052   fscanf(fp, "%s %d",  dummy, &stepDump);
00053   fscanf(fp, "%s %d",  dummy, &stepTraj);
00054   fscanf(fp, "%s %d",  dummy, &limitCorrAv);
00055   fscanf(fp, "%s %d",  dummy, &nBuffCorr);
00056   fscanf(fp, "%s %d",  dummy, &nFunCorr);
00057   fscanf(fp, "%s %d",  dummy, &nValCorr);
00058   fscanf(fp, "%s %d",  dummy, &stepCorr);
00059   fscanf(fp, "%s %d",  dummy, &limitAcfAv);
```

```
00060   fscanf(fp, "%s %d",  dummy, &nBuffAcf);
00061   fscanf(fp, "%s %d",  dummy, &nValAcf);
00062   fscanf(fp, "%s %d",  dummy, &stepAcf);
00063   fscanf(fp, "%s %lf", dummy, &rangeRdf);
00064   fscanf(fp, "%s %d",  dummy, &limitRdf);
00065   fscanf(fp, "%s %d",  dummy, &sizeHistRdf);
00066   fscanf(fp, "%s %d",  dummy, &stepRdf);
00067
00068   fclose(fp);
00069   FILE *fpSTATE;
00070   if((fpSTATE = fopen(inputConfig,"r"))==NULL){
00071   printf("Error occurred: Could not open STATE file\n Exiting now..\n");
00072   exit(0);
00073   }
00074
00075   fscanf(fpSTATE, "%s %lf", dummy, &timeNow);
00076   fscanf(fpSTATE, "%s %d",  dummy, &nAtom);
00077   fscanf(fpSTATE, "%s %d",  dummy, &nBond);
00078   fscanf(fpSTATE, "%s %d",  dummy, &nAtomType);
00079   fscanf(fpSTATE, "%s %d",  dummy, &nBondType);
00080   fscanf(fpSTATE, "%s %lf", dummy, &region[1]);
00081   fscanf(fpSTATE, "%s %lf", dummy, &region[2]);
00082
00083   region[2] *= 1.5; //Remove this when put on GitHub
00084
00085   density = nAtom/(region[1]*region[2]);
00086   cells[1] = region[1] / rCut;
00087   cells[2] = region[2] / rCut;
00088   cellList = (int*)malloc((nAtom + cells[1] * cells[2] + 1) * sizeof(int));
00089   regionH[1] = 0.5*region[1];
00090   regionH[2] = 0.5*region[2];
00091
00092   //strain information
00093   strainRate = strain/deltaT;
00094   shearDisplacement = strain * region[2];
00095   shearVelocity = strainRate * region[2];
00096   int n;
00097
00098   rx = (double*)malloc((nAtom + 1) * sizeof(double));
00099   ry = (double*)malloc((nAtom + 1) * sizeof(double));
00100   vx = (double*)malloc((nAtom + 1) * sizeof(double));
00101   vy = (double*)malloc((nAtom + 1) * sizeof(double));
00102   ax = (double*)malloc((nAtom + 1) * sizeof(double));
00103   ay = (double*)malloc((nAtom + 1) * sizeof(double));
00104   fax = (double*)malloc((nAtom + 1) * sizeof(double));
00105   fay = (double*)malloc((nAtom + 1) * sizeof(double));
00106   atomID = (int*)malloc((nAtom+1) * sizeof(int));
00107   atomType = (int*)malloc((nAtom+1) * sizeof(int));
00108   atomRadius = (double*)malloc((nAtom + 1) * sizeof(double));
00109   atomMass = (double*)malloc((nAtom + 1) * sizeof(double));
00110   speed = (double*)malloc((nAtom + 1) * sizeof(double));
00111   atom1 = (int*)malloc((nBond+1)*sizeof(int));
00112   atom2 = (int*)malloc((nBond+1)*sizeof(int));
00113   BondID = (int*)malloc((nBond+1)*sizeof(int));
00114   BondType = (int*)malloc((nBond+1)*sizeof(int));
00115   kb = (double*)malloc((nBond+1)*sizeof(double));
00116   ro = (double*)malloc((nBond+1)*sizeof(double));
00117   BondEnergy = (double*)malloc((nBond+1)*sizeof(double));
00118   BondLength =(double*)malloc((nBond+1)*sizeof(double));
00119   discDragx = (double*)malloc((nAtom + 1) * sizeof(double));
00120   discDragy = (double*)malloc((nAtom + 1) * sizeof(double));
00121   nodeDragx = (double*)malloc((nAtom + 1) * sizeof(double));
00122   nodeDragy = (double*)malloc((nAtom + 1) * sizeof(double));
00123   ImageX = (int*)malloc((nAtom+1) * sizeof(int));
00124   ImageY = (int*)malloc((nAtom+1) * sizeof(int));
00125   rxUnwrap = (double*)malloc((nAtom + 1) * sizeof(double));
00126   ryUnwrap = (double*)malloc((nAtom + 1) * sizeof(double));
00127   DeltaXijOld = (double*)malloc((nBond+1)*sizeof(double));
00128   DeltaYijOld = (double*)malloc((nBond+1)*sizeof(double));
00129   DeltaXijOldPair = (double**)malloc((nAtom+1) * sizeof(double*));
00130   DeltaYijOldPair = (double**)malloc((nAtom+1) * sizeof(double*));
00131   for(int n = 0; n <= nAtom; n++) {
00132    DeltaXijOldPair[n] = (double*)malloc((nAtom+1) * sizeof(double));
00133    DeltaYijOldPair[n] = (double*)malloc((nAtom+1) * sizeof(double));
00134   }
00135   molID = (int*)malloc((nAtom+1) * sizeof(int));
00136
00137   for(n = 1; n <= nAtom; n ++){
00138    atomMass[n] = 1.0;
00139   }
00140
00141   fscanf(fpSTATE, "%s\n", dummy);
00142   for(n = 1; n <= nAtom; n ++)
00143    fscanf(fpSTATE, "%d %d %d %lf %lf %lf %lf %lf\n", &atomID[n], &molID[n], &atomType[n],
      &atomRadius[n], &rx[n], &ry[n], &vx[n], &vy[n]);
00144
00145
```

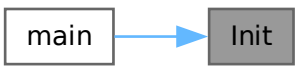
```
00146   fscanf(fpSTATE, "%s\n", dummy);
00147   for(n=1; n<=nBond; n++)
00148    fscanf(fpSTATE, "%d %d %d %d %lf %lf\n", &BondID[n], &BondType[n], &atom1[n], &atom2[n], &kb[n],
      &ro[n]);
00149
00150   fclose(fpSTATE);
00151
00152  //2D-List of bonded atoms. This is used to remove pair interaction
00153  //calculation for the bonded atoms
00154    isBonded = (int**)malloc((nAtom + 1) * sizeof(int*));
00155   for (int i = 0; i <= nAtom; i++) {
00156     isBonded[i] = (int*)malloc((nAtom + 1) * sizeof(int));
00157     for (int j = 0; j <= nAtom; j++) {
00158         isBonded[i][j] = 0;
00159     }
00160   }
00161
00162   for (n = 1; n <= nBond; n++) {
00163     int i = atom1[n];
00164     int j = atom2[n];
00165     isBonded[i][j] = 1;
00166     isBonded[j][i] = 1; // symmetric
00167 }
00168
00169  //For thermostate, update in final version
00170 thermo = 'C';
00171
00172
00173  // List the interface atoms
00174  nAtomInterface = 0;
00175  nAtomBlock = 0;
00176  nDiscInterface = 0;
00177  double InterfaceWidth, bigDiameter;
00178  bigDiameter = 2.8;
00179  InterfaceWidth = 5.0 * bigDiameter;
00180
00181  for(n = 1; n <= nAtom; n++){
00182   if(fabs(ry[n]) < InterfaceWidth){
00183   nAtomInterface++;
00184   }
00185   if(molID[n] == 2){
00186   nAtomBlock++;
00187   }
00188   if(atomRadius[n] != 0.0){
00189   nDiscInterface++;
00190   } }
00191
00192    atomIDInterface =  (int*)malloc((nAtomInterface+1)*sizeof(int));
00193
00194   int m;
00195   m = 1;
00196   for(n=1; n<=nAtom; n++){
00197    if(fabs(ry[n]) < InterfaceWidth){
00198    atomIDInterface[m] = atomID[n];
00199    m++;
00200    } }
00201
00202   nPairTotal = 0.5 * nAtomInterface * (nAtomInterface-1);
00203   PairID = (int*)malloc((nPairTotal+1) * sizeof(int));
00204   Pairatom1 = (int*)malloc((nPairTotal+1) * sizeof(int));
00205   Pairatom2 = (int*)malloc((nPairTotal+1) * sizeof(int));
00206   PairXij = (double*)malloc((nPairTotal+1) * sizeof(double));
00207   PairYij = (double*)malloc((nPairTotal+1) * sizeof(double));
00208
00209     fprintf(fpresult, "-------------------------------------\n");
00210     fprintf(fpresult, "-------PARAMETERS-----------\n");
00211     fprintf(fpresult, "-------------------------------------\n");
00212     fprintf(fpresult, "nAtom\t\t\t%d\n",  nAtom);
00213     fprintf(fpresult, "nBond\t\t\t%d\n",  nBond);
00214     fprintf(fpresult, "nAtomBlock\t\t%d\n",  nAtomBlock);
00215     fprintf(fpresult, "nAtomInterface\t%d\n",  nAtomInterface);
00216     fprintf(fpresult, "nDiscInterface\t\t%d\n",  nDiscInterface);
00217     fprintf(fpresult, "gamman\t\t\t%0.6g\n", gamman);
00218     fprintf(fpresult, "strain\t\t\t%0.6g\n", strain);
00219     fprintf(fpresult, "strainRate\t\t%0.6g\n", strainRate);
00220     fprintf(fpresult, "FyBylx\t\t\t%0.6g\n", FyBylx);
00221     fprintf(fpresult, "fxByfy\t\t\t%0.6g\n", fxByfy);
00222     fprintf(fpresult, "DeltaY\t\t\t%0.6g\n", DeltaY);
00223     fprintf(fpresult, "DeltaX\t\t\t%0.6g\n", DeltaX);
00224     fprintf(fpresult, "HaltCondition\t\t%0.6g\n", HaltCondition);
00225     fprintf(fpresult, "kappa\t\t\t%g\n", kappa);
00226     fprintf(fpresult, "density\t\t\t%g\n", density);
00227     fprintf(fpresult, "rCut\t\t\t%g\n", rCut);
00228     fprintf(fpresult, "deltaT\t\t\t%g\n", deltaT);
00229     fprintf(fpresult, "stepEquil\t\t\t%d\n",  stepEquil);
00230     fprintf(fpresult, "stepLimit\t\t\t%d\n",  stepLimit);
00231     fprintf(fpresult, "region[1]\t\t\t%0.16lf\n", region[1]);
```

```
00232     fprintf(fpresult, "region[2]\t\t\t%0.16lf\n", region[2]);
00233     fprintf(fpresult, "cells[1]\t\t\t%d\n",  cells[1]);
00234     fprintf(fpresult, "cells[2]\t\t\t%d\n",  cells[2]);
00235     fprintf(fpresult, "solver\t\t\t%s\n",  solver);
00236     fprintf(fpresult, "boundary\t\t\t%s %s\n", xBoundary, yBoundary);
00237     fprintf(fpresult, "DampFlag\t\t%d\n",  DampFlag);
00238
00239
00240     fprintf(fpresult, "-----------------------------------\n");
00241     fprintf(fpresult, "#TimeNow TotalMomentum PotEngyPerAtom KinEngyPerAtom TotEngyPerAtom
      PairEnergyPerAtom BondEnergyPerAtom  Press VirialSum\n");
00242     fprintf(fpvrms, "#timeNow\tVrms \n");
00243     fprintf(fpcom, "#timeNow\tComX\tComY\n");
00244
00245 /* //Uncomment the following as per your acquirement
00246     fprintf(fpstress, "strain           %lf\n", strain);
00247     fprintf(fpstress, "region[1]        %lf\n", region[1]);
00248     fprintf(fpstress, "region[2]        %lf\n", region[2]);
00249     fprintf(fpstress, "#timeNow virSumxx virSumyy virSumxy pressure\n");
00250     fprintf(fpmomentum, "#timeNow Px Py\n");
00251 */
00252
00253    if((strcmp(xBoundary, "p") != 0 && strcmp(xBoundary, "r") != 0) ||
00254     (strcmp(yBoundary, "p") != 0 && strcmp(yBoundary, "r") != 0)) {
00255     fprintf(fpresult, "Error: Invalid boundary value detected: '%s %s'. Only 'p' or 'r' are
      allowed.\n", xBoundary, yBoundary);
00256     exit(EXIT_FAILURE); // Exit with failure status
00257   }
00258
00259 }
```

References atom1, atom2, atomID, atomIDInterface, atomMass, atomRadius, atomType, ax, ay, BondEnergy, BondID, BondLength, BondType, cellList, cells, DampFlag, deltaT, DeltaX, DeltaXijOld, DeltaXijOldPair, DeltaY, DeltaYijOld, DeltaYijOldPair, density, discDragx, discDragy, fax, fay, fpcom, fpresult, fpvrms, freezeAtomType, fxByfy, FyBylx, gamman, HaltCondition, ImageX, ImageY, isBonded, kappa, kb, limitAcfAv, limitCorrAv, limitRdf, molID, nAtom, nAtomBlock, nAtomInterface, nAtomType, nBond, nBondType, nBuffAcf, nBuffCorr, nDiscInterface, nFunCorr, nodeDragx, nodeDragy, nPairTotal, nValAcf, nValCorr, Pairatom1, Pairatom2, PairID, PairXij, PairYij, rangeRdf, rCut, region, regionH, ro, rx, rxUnwrap, ry, ryUnwrap, shearDisplacement, shearVelocity, sizeHistRdf, solver, speed, stepAcf, stepAvg, stepCorr, stepDump, stepEquil, stepLimit, stepRdf, stepTraj, strain, strainRate, thermo, timeNow, vx, vy, xBoundary, and yBoundary.

Referenced by main().

Here is the caller graph for this function:



3.72.2.25 LeapfrogStep()

```
void LeapfrogStep ( )
```

3.72.2.26 main()

```
int main (
            int argc,
            char ** argv )
```

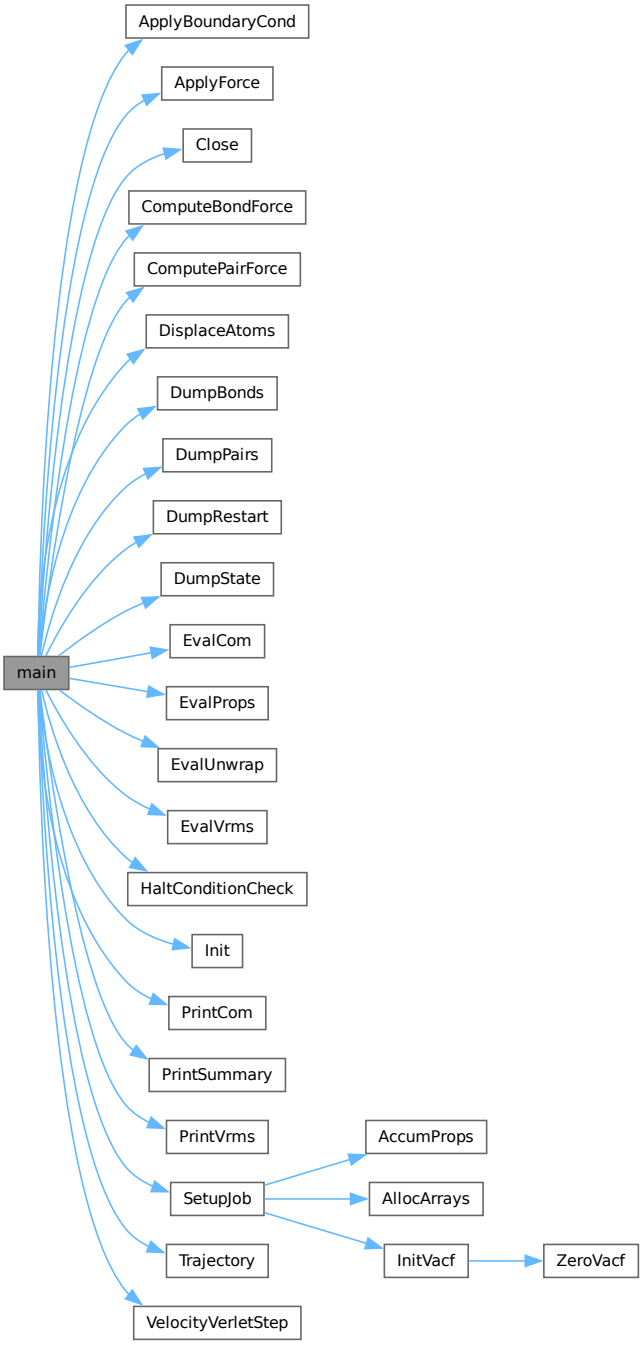
Definition at line 51 of file main.c.

```
00051                                {
00052  time_t t1 = 0, t2;
00053  if (argc < 2) {
00054  fprintf(stderr, "Usage: %s <output_prefix>\n", argv[0]);
00055  return 1;
00056  }
00057   int prefix_size = snprintf(NULL, 0, "../output/%s", argv[1]) + 1; // +1 for the null terminator
00058   prefix = malloc(prefix_size);
00059   if(prefix == NULL) {
00060    fprintf(stderr, "Memory allocation failed\n");
00061    return 1;
00062    }
00063
00064    // Write the formatted string into the allocated space
00065   snprintf(prefix, prefix_size, "../output/%s", argv[1]);
00066   sprintf(result, "%s.result", prefix);
00067   fpresult = fopen(result, "w");
00068   sprintf(xyz, "%s.xyz", prefix);
00069   fpxyz = fopen(xyz, "w");
00070   sprintf(vrms, "%s.vrms", prefix);
00071   fpvrms = fopen(vrms, "w");
00072   sprintf(bond, "%s.bond", prefix);
00073   fpbond = fopen(bond, "w");
00074   sprintf(com, "%s.com", prefix);
00075   fpcom = fopen(com, "w");
00076   sprintf(pair, "%s.pair", prefix);
00077   fppair = fopen(pair, "w");
00078
00079   /* //Uncomment the following as per your acquirement
00080   sprintf(dnsty, "%s.curr-dnsty", prefix);
00081   fpdnsty = fopen(dnsty, "w");
00082   sprintf(visc, "%s.viscosity", prefix);
00083   fpvisc = fopen(visc, "w");
00084   sprintf(rdf, "%s.rdf", prefix);
00085   fprdf = fopen(rdf, "w");
00086   sprintf(stress, "%s.stress", prefix);
00087   fpstress = fopen(stress, "w");
00088   sprintf(momentum, "%s.momentum", prefix);
00089   fpmomentum = fopen(momentum, "w");
00090   */
00091
00092   Init();
00093   SetupJob();
00094   t1 = time(NULL);
00095   moreCycles = 1;
00096   timeNow = 0.0;
00097   if(timeNow == 0.0) {
00098    DisplaceAtoms();
00099    ComputePairForce(1);
00100    ComputeBondForce();
00101    ApplyForce();
00102    DumpBonds();
00103    DumpPairs();
00104    Trajectory();
00105    EvalUnwrap();
00106    ApplyBoundaryCond();
00107    EvalProps();
00108    EvalVrms();
00109    EvalCom();
00110    PrintVrms();
00111    PrintCom();
00112    PrintSummary();
00113    }
00114
00115 //Here starts the main loop of the program
00116   while(moreCycles){
00117    if(stepLimit == 0){
00118    exit(0);
00119    }
00120
00121    stepCount ++;
00122    timeNow = stepCount * deltaT; //for adaptive step size: timeNow += deltaT
00123
00124    VelocityVerletStep(1);
00125    EvalUnwrap();
00126    ApplyBoundaryCond();
00127    ComputePairForce(1);
00128    ComputeBondForce();
00129    ApplyForce();
00130    VelocityVerletStep(2);
00131    ApplyBoundaryCond();
00132    EvalProps();
00133    EvalVrms();
00134    EvalCom();
00135    if(stepCount % stepAvg == 0){
00136     PrintSummary();
```

```
00137     PrintVrms();
00138     PrintCom();
00139     }
00140    if(stepCount % stepTraj == 0){
00141     Trajectory();
00142     DumpBonds();
00143     DumpPairs();
00144     }
00145    if(stepCount % stepDump == 0){
00146     DumpRestart();      // Save the current state for input
00147     DumpState();        // Save the current state for config
00148    }
00149    if(HaltConditionCheck(VRootMeanSqr, stepCount)) {
00150     DumpRestart();      // Save the current state for input
00151     DumpState();        // Save the current state for config
00152     break;  // Exit the loop when the halt condition is met
00153     }
00154
00155     if(stepCount >= stepLimit)
00156      moreCycles = 0;
00157   }
00158
00159
00160   t2 = time(NULL);
00161   fprintf(fpresult, "#Execution time %lf secs\n", difftime(t2,t1));
00162   fprintf(fpresult, "#Execution speed %lf steps per secs\n", stepLimit/difftime(t2,t1));
00163
00164   fclose(fpresult);
00165   fclose(fpxyz);
00166   fclose(fpvrms);
00167   fclose(fpbond);
00168   fclose(fppair);
00169   fclose(fpcom);
00170
00171 /*//Uncomment the following as per your acquirement
00172   fclose(fpdnsty);
00173   fclose(fpvisc);
00174   fclose(fprdf);
00175   fclose(fpstress);
00176   fclose(fpmomentum);
00177 */
00178
00179   free(prefix);
00180   Close();
00181   return 0;
00182 }
```

References ApplyBoundaryCond(), ApplyForce(), bond, Close(), com, ComputeBondForce(), ComputePairForce(), deltaT, DisplaceAtoms(), DumpBonds(), DumpPairs(), DumpRestart(), DumpState(), EvalCom(), EvalProps(), EvalUnwrap(), EvalVrms(), fpbond, fpcom, fppair, fpresult, fpvrms, fpxyz, HaltConditionCheck(), Init(), moreCycles, pair, prefix, PrintCom(), PrintSummary(), PrintVrms(), result, SetupJob(), stepAvg, stepCount, stepDump, stepLimit, stepTraj, timeNow, Trajectory(), VelocityVerletStep(), vrms, VRootMeanSqr, and xyz.

Here is the call graph for this function:



3.72.2.27 PrintCom()

```
void PrintCom ( )
```

Definition at line 28 of file PrintCom.c.

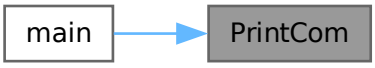
```
00028                   {
```

```
00029  fprintf(fpcom, "%0.4lf\t%0.16lf\t%0.16lf\n", timeNow, ComX, ComY);
00030  fflush(fpcom);
00031  }
```

References ComX, ComY, fpcom, and timeNow.

Referenced by main().

Here is the caller graph for this function:



3.72.2.28 PrintMomentum()

```
void PrintMomentum ( )
```

Definition at line 25 of file PrintMomentum.c.

```
00025                    {
00026  fprintf(fpmomentum, "%0.4lf\t%0.16lf\t%0.16lf\n", timeNow, vSumX, vSumY);
00027  fflush(fpmomentum);
00028 }
```

References fpmomentum, timeNow, vSumX, and vSumY.

3.72.2.29 PrintStress()

```
void PrintStress ( )
```

Definition at line 25 of file PrintStress.c.

```
00025                   {
00026   fprintf(fpstress, "%0.4lf\t%0.16lf\t%0.16lf\t%0.16lf\t%0.16lf\n", timeNow, virSumxx, virSumyy,
      virSumxy, pressure);
00027   fflush(fpstress);
00028 }
```

References fpstress, pressure, timeNow, virSumxx, virSumxy, and virSumyy.

3.72.2.30 PrintSummary()

```
void PrintSummary ( )
```

Definition at line 4 of file PrintSummary.c.

```
00004                   {
00005   fprintf(fpresult, "%0.4lf\t%0.16lf\t%0.16lf\t%0.16lf\t%0.16lf\t%0.16lf\t%0.16lf\t%0.16lf\n",
00006    timeNow, vSum, potEnergy, kinEnergy, totEnergy, uSumPairPerAtom, BondEnergyPerAtom, pressure,
       virSum);
00007    fflush(fpresult);
00008 }
```

References BondEnergyPerAtom, fpresult, kinEnergy, potEnergy, pressure, timeNow, totEnergy, uSumPairPerAtom, virSum, and vSum.

Referenced by main().

Here is the caller graph for this function:

3.72.2.31 PrintVrms()

```
void PrintVrms ( )
```

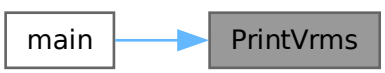
Definition at line 27 of file PrintVrms.c.

```
00027                 {
00028   fprintf(fpvrms, "%0.4lf\t%0.16lf\n", timeNow, VRootMeanSqr);
00029   fflush(fpvrms);
00030 }
```

References fpvrms, timeNow, and VRootMeanSqr.

Referenced by main().

Here is the caller graph for this function:



3.72.2.32 SetupJob()

```
void SetupJob ( )
```

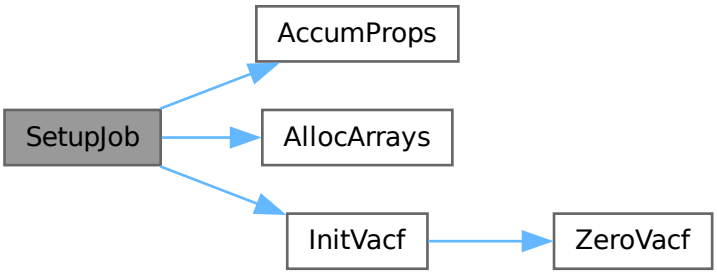
Definition at line 27 of file SetupJob.c.

```
00027               {
00028   AllocArrays();
00029   AccumProps(0);
00030   InitVacf();
00031   stepCount = 0;
00032   // INITIALISE SPACETIME CORRELATIONS
00033   int n;
00034   for (n = 1; n <= nBuffCorr; n++)
00035     indexCorr[n] = -(n - 1)*nValCorr/nBuffCorr;
00036
00037   countCorrAv = 0.;
00038
00039   for (n = 1; n <= nFunCorr*nValCorr; n++)
00040     spacetimeCorrAv[n] = 0.;
00041
00042   //RDF
00043   countRdf = 0;
00044 }
```

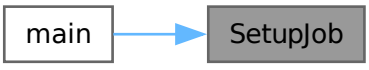
References AccumProps(), AllocArrays(), countCorrAv, countRdf, indexCorr, InitVacf(), nBuffCorr, nFunCorr, nValCorr, spacetimeCorrAv, and stepCount.

Referenced by main().

Here is the call graph for this function:



Here is the caller graph for this function:



3.72.2.33 Trajectory()

```
void Trajectory ( )
```

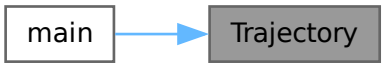
Definition at line 25 of file Trajectory.c.

```
00025                {
00026  int n;
00027  //Trajectory file in LAMMPS dump format for OVITO visualization
00028  fprintf(fpxyz, "ITEM: TIMESTEP\n");
00029  fprintf(fpxyz, "%lf\n",timeNow);
00030  fprintf(fpxyz, "ITEM: NUMBER OF ATOMS\n");
00031  fprintf(fpxyz, "%d\n",nAtom);
00032  fprintf(fpxyz, "ITEM: BOX BOUNDS pp ff pp\n");
00033  fprintf(fpxyz, "%lf %lf xlo xhi\n", -regionH[1], regionH[1]);
00034  fprintf(fpxyz, "%lf %lf ylo yhi\n", -regionH[2], regionH[2]);
00035  fprintf(fpxyz, "%lf %lf zlo zhi\n", -0.1, 0.1);
00036  fprintf(fpxyz, "ITEM: ATOMS id mol type radius x y vx vy fx fy\n");
00037  for(n=1; n<=nAtom; n++)
00038   fprintf(fpxyz, "%d\t %d\t %d\t %0.2lf\t %0.16lf\t %0.16lf\t %0.16lf\t %0.16lf\t %0.16lf\t
      %0.16lf\n",
00039   atomID[n], molID[n], atomType[n], atomRadius[n], rx[n], ry[n], vx[n], vy[n], ax[n], ay[n]);
00040 }
```

References atomID, atomRadius, atomType, ax, ay, fpxyz, molID, nAtom, regionH, rx, ry, timeNow, vx, and vy.

Referenced by main().

Here is the caller graph for this function:



3.72.2.34 VelocityVerletStep()

```
void VelocityVerletStep (
             int icode )
```

Definition at line 26 of file VelocityVerletStep.c.

```
00026                                {
00027 int n;
00028  if(icode == 1){
00029  for (n= 1; n <= nAtom; n++) {
00030   if(atomType[n] != freezeAtomType){
00031   vx[n] += ax[n] * 0.5 * deltaT;
00032   vy[n] += ay[n] * 0.5 * deltaT;
00033   rx[n] += vx[n] * deltaT;
00034   ry[n] += vy[n] * deltaT;
00035   }
00036   //Calculating the image flags here
00037   if (rx[n] >= regionH[1]) {
00038    rx[n] -= region[1];
00039    ImageX[n]++;
00040    } else if (rx[n] < -regionH[1]) {
00041    rx[n] += region[1];
00042   ImageX[n]--;
00043   }
00044   if (ry[n] >= regionH[2]) {
00045    ry[n] -= region[2];
00046    ImageY[n]++;
00047    } else if (ry[n] < -regionH[2]) {
00048    ry[n] += region[2];
```

```
00049     ImageY[n]--;
00050     } } }
00051    else if(icode == 2){
00052    for(n = 1; n <= nAtom; n++) {
00053    if(atomType[n] != freezeAtomType){
00054     vx[n] += ax[n] * 0.5 * deltaT;
00055     vy[n] += ay[n] * 0.5 * deltaT;
00056 } } } }
```

References atomType, ax, ay, deltaT, freezeAtomType, ImageX, ImageY, nAtom, region, regionH, rx, ry, vx, and vy.

Referenced by main().

Here is the caller graph for this function:

3.72.3 Variable Documentation

3.72.3.1 prefix

```
char* prefix = NULL
```

Definition at line 13 of file main.c.

Referenced by DumpRestart(), DumpState(), and main().

3.73 main.c

Go to the documentation of this file.

```
00001 #include<stdio.h>
00002 #include<string.h>
00003 #include<stdlib.h>
00004 #include <stdbool.h>
00005 #include <time.h>
00006 #include <mpi.h>
00007 #define DEFINE_GLOBALS
00008 #include "global.h"
00009 #include "ComputeBondForce.h"
00010 #include "ComputePairForce.h"
00011
00012
00013 char *prefix = NULL;  // Definition of prefix
00014
00015 void Init();
00016 void SetupJob();
00017 void EvalSpacetimeCorr();
00018 void Trajectory();
00019 void DumpState();
00020 void ComputeForcesCells();
00021 void LeapfrogStep();
00022 void BrownianStep();
00023 void ApplyBoundaryCond();
00024 void EvalProps();
00025 void EvalVacf();
```

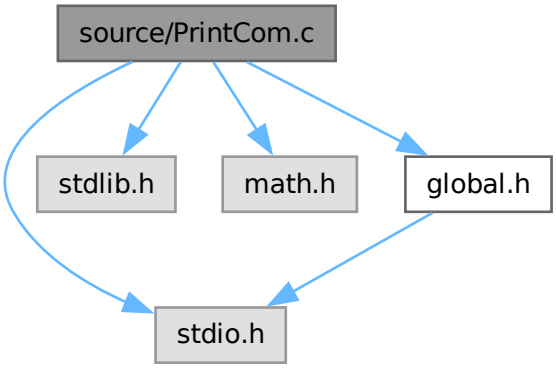
```
00026 void EvalRdf();
00027 void AccumProps(int icode);
00028 void PrintSummary();
00029 void PrintVrms();
00030 //void ComputeBondForce();
00031 void DumpBonds();
00032 void VelocityVerletStep(int icode);
00033 void ApplyForce();
00034 void ApplyDrivingForce();
00035 void ApplyShear();
00036 void ApplyLeesEdwardsBoundaryCond();
00037 void PrintStress();
00038 void Close();
00039 //void ComputePairForce(int normFlag);
00040 void PrintMomentum();
00041 void DisplaceAtoms();
00042 void DumpRestart();
00043 bool HaltConditionCheck(double value, int stepCount);
00044 void EvalCom();
00045 void PrintCom();
00046 void EvalVrms();
00047 void EvalUnwrap();
00048 void DumpPairs();
00049 void ApplyViscous();
00050
00051 int main(int argc, char **argv) {
00052  time_t t1 = 0, t2;
00053  if (argc < 2) {
00054  fprintf(stderr, "Usage: %s <output_prefix>\n", argv[0]);
00055  return 1;
00056  }
00057   int prefix_size = snprintf(NULL, 0, "../output/%s", argv[1]) + 1; // +1 for the null terminator
00058   prefix = malloc(prefix_size);
00059   if(prefix == NULL) {
00060    fprintf(stderr, "Memory allocation failed\n");
00061    return 1;
00062    }
00063
00064    // Write the formatted string into the allocated space
00065   snprintf(prefix, prefix_size, "../output/%s", argv[1]);
00066   sprintf(result, "%s.result", prefix);
00067   fpresult = fopen(result, "w");
00068   sprintf(xyz, "%s.xyz", prefix);
00069   fpxyz = fopen(xyz, "w");
00070   sprintf(vrms, "%s.vrms", prefix);
00071   fpvrms = fopen(vrms, "w");
00072   sprintf(bond, "%s.bond", prefix);
00073   fpbond = fopen(bond, "w");
00074   sprintf(com, "%s.com", prefix);
00075   fpcom = fopen(com, "w");
00076   sprintf(pair, "%s.pair", prefix);
00077   fppair = fopen(pair, "w");
00078
00079   /* //Uncomment the following as per your acquirement
00080   sprintf(dnsty, "%s.curr-dnsty", prefix);
00081   fpdnsty = fopen(dnsty, "w");
00082   sprintf(visc, "%s.viscosity", prefix);
00083   fpvisc = fopen(visc, "w");
00084   sprintf(rdf, "%s.rdf", prefix);
00085   fprdf = fopen(rdf, "w");
00086   sprintf(stress, "%s.stress", prefix);
00087   fpstress = fopen(stress, "w");
00088   sprintf(momentum, "%s.momentum", prefix);
00089   fpmomentum = fopen(momentum, "w");
00090   */
00091
00092   Init();
00093   SetupJob();
00094   t1 = time(NULL);
00095   moreCycles = 1;
00096   timeNow = 0.0;
00097   if(timeNow == 0.0) {
00098    DisplaceAtoms();
00099    ComputePairForce(1);
00100    ComputeBondForce();
00101    ApplyForce();
00102    DumpBonds();
00103    DumpPairs();
00104    Trajectory();
00105    EvalUnwrap();
00106    ApplyBoundaryCond();
00107    EvalProps();
00108    EvalVrms();
00109    EvalCom();
00110    PrintVrms();
00111    PrintCom();
00112    PrintSummary();
```

```
00113    }
00114
00115 //Here starts the main loop of the program
00116   while(moreCycles){
00117    if(stepLimit == 0){
00118    exit(0);
00119    }
00120
00121    stepCount ++;
00122    timeNow = stepCount * deltaT; //for adaptive step size: timeNow += deltaT
00123
00124    VelocityVerletStep(1);
00125    EvalUnwrap();
00126    ApplyBoundaryCond();
00127    ComputePairForce(1);
00128    ComputeBondForce();
00129    ApplyForce();
00130    VelocityVerletStep(2);
00131    ApplyBoundaryCond();
00132    EvalProps();
00133    EvalVrms();
00134    EvalCom();
00135    if(stepCount % stepAvg == 0){
00136     PrintSummary();
00137     PrintVrms();
00138     PrintCom();
00139     }
00140    if(stepCount % stepTraj == 0){
00141     Trajectory();
00142     DumpBonds();
00143     DumpPairs();
00144     }
00145    if(stepCount % stepDump == 0){
00146     DumpRestart();     // Save the current state for input
00147     DumpState();       // Save the current state for config
00148    }
00149    if(HaltConditionCheck(VRootMeanSqr, stepCount)) {
00150     DumpRestart();     // Save the current state for input
00151     DumpState();       // Save the current state for config
00152     break;  // Exit the loop when the halt condition is met
00153     }
00154
00155     if(stepCount >= stepLimit)
00156      moreCycles = 0;
00157   }
00158
00159
00160   t2 = time(NULL);
00161   fprintf(fpresult, "#Execution time %lf secs\n", difftime(t2,t1));
00162   fprintf(fpresult, "#Execution speed %lf steps per secs\n", stepLimit/difftime(t2,t1));
00163
00164   fclose(fpresult);
00165   fclose(fpxyz);
00166   fclose(fpvrms);
00167   fclose(fpbond);
00168   fclose(fppair);
00169   fclose(fpcom);
00170
00171 /*//Uncomment the following as per your acquirement
00172   fclose(fpdnsty);
00173   fclose(fpvisc);
00174   fclose(fprdf);
00175   fclose(fpstress);
00176   fclose(fpmomentum);
00177 */
00178
00179   free(prefix);
00180   Close();
00181   return 0;
00182 }
```

3.74 source/PrintCom.c File Reference

```
#include <stdio.h>
#include <stdlib.h>
#include <math.h>
#include "global.h"
```

Include dependency graph for PrintCom.c:



Functions

- void PrintCom ()

3.74.1 Function Documentation

3.74.1.1 PrintCom()

```
void PrintCom ( )
```

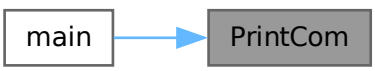
Definition at line 28 of file PrintCom.c.

```
00028                 {
00029   fprintf(fpcom, "%0.4lf\t%0.16lf\t%0.16lf\n", timeNow, ComX, ComY);
00030   fflush(fpcom);
00031   }
```

References ComX, ComY, fpcom, and timeNow.

Referenced by main().

Here is the caller graph for this function:



3.75 PrintCom.c

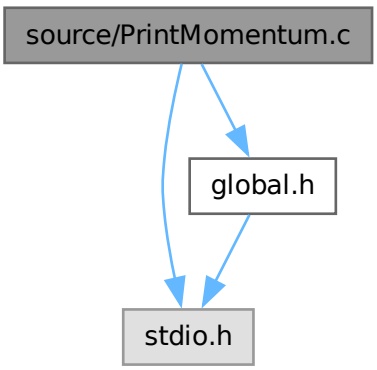
Go to the documentation of this file.

```
00001 /*
00002  * This file is part of Lamina.
00003  *
00004  * Lamina is free software: you can redistribute it and/or modify
00005  * it under the terms of the GNU General Public License as published by
00006  * the Free Software Foundation, either version 3 of the License, or
00007  * (at your option) any later version.
00008  *
00009  * Lamina is distributed in the hope that it will be useful,
00010  * but WITHOUT ANY WARRANTY; without even the implied warranty of
00011  * MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the
00012  * GNU General Public License for more details.
00013  *
00014  * You should have received a copy of the GNU General Public License
00015  * along with Lamina. If not, see <https://www.gnu.org/licenses/>.
00016
00017  Copyright (C) 2025 Harish Charan, University of Durham, UK
00018
00019  */
00020
00021
00022
00023 #include<stdio.h>
00024 #include<stdlib.h>
00025 #include<math.h>
00026 #include"global.h"
00027
00028 void PrintCom(){
00029  fprintf(fpcom, "%0.4lf\t%0.16lf\t%0.16lf\n", timeNow, ComX, ComY);
00030  fflush(fpcom);
00031  }
00032
00033
00034
```

3.76 source/PrintMomentum.c File Reference

```
#include <stdio.h>
#include "global.h"
```

Include dependency graph for PrintMomentum.c:



Functions

- void PrintMomentum ()

3.76.1 Function Documentation

3.76.1.1 PrintMomentum()

```
void PrintMomentum ( )
```

Definition at line 25 of file PrintMomentum.c.

```
00025                    {
00026  fprintf(fpmomentum, "%0.4lf\t%0.16lf\t%0.16lf\n", timeNow, vSumX, vSumY);
00027  fflush(fpmomentum);
00028 }
```

References fpmomentum, timeNow, vSumX, and vSumY.

3.77 PrintMomentum.c

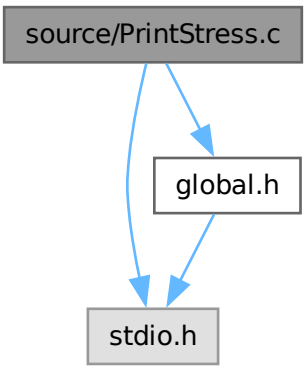
Go to the documentation of this file.

```
00001 /*
00002  * This file is part of Lamina.
00003  *
00004  * Lamina is free software: you can redistribute it and/or modify
00005  * it under the terms of the GNU General Public License as published by
00006  * the Free Software Foundation, either version 3 of the License, or
00007  * (at your option) any later version.
00008  *
00009  * Lamina is distributed in the hope that it will be useful,
00010  * but WITHOUT ANY WARRANTY; without even the implied warranty of
00011  * MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the
00012  * GNU General Public License for more details.
00013  *
00014  * You should have received a copy of the GNU General Public License
00015  * along with Lamina. If not, see <https://www.gnu.org/licenses/>.
00016
00017  Copyright (C) 2025 Harish Charan, University of Durham, UK
00018
00019  */
00020
00021
00022 #include<stdio.h>
00023 #include"global.h"
00024
00025 void PrintMomentum(){
00026  fprintf(fpmomentum, "%0.4lf\t%0.16lf\t%0.16lf\n", timeNow, vSumX, vSumY);
00027  fflush(fpmomentum);
00028 }
```

3.78 source/PrintStress.c File Reference

```
#include <stdio.h>
#include "global.h"
```

Include dependency graph for PrintStress.c:



Functions

- void PrintStress ()

3.78.1 Function Documentation

3.78.1.1 PrintStress()

```
void PrintStress ( )
```

Definition at line 25 of file PrintStress.c.

```
00025                   {
00026   fprintf(fpstress, "%0.4lf\t%0.16lf\t%0.16lf\t%0.16lf\t%0.16lf\n", timeNow, virSumxx, virSumyy,
      virSumxy, pressure);
00027   fflush(fpstress);
00028 }
```

References fpstress, pressure, timeNow, virSumxx, virSumxy, and virSumyy.

3.79 PrintStress.c

Go to the documentation of this file.

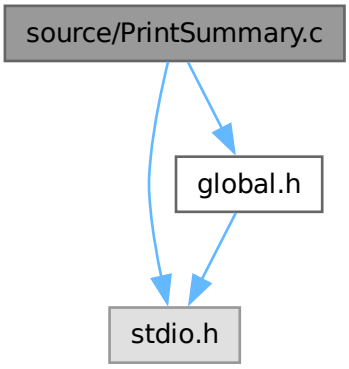
```
00001 /*
00002  * This file is part of Lamina.
00003  *
00004  * Lamina is free software: you can redistribute it and/or modify
00005  * it under the terms of the GNU General Public License as published by
00006  * the Free Software Foundation, either version 3 of the License, or
00007  * (at your option) any later version.
00008  *
00009  * Lamina is distributed in the hope that it will be useful,
00010  * but WITHOUT ANY WARRANTY; without even the implied warranty of
00011  * MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the
00012  * GNU General Public License for more details.
00013  *
00014  * You should have received a copy of the GNU General Public License
00015  * along with Lamina. If not, see <https://www.gnu.org/licenses/>.
```

```
00016
00017  Copyright (C) 2025 Harish Charan, University of Durham, UK
00018
00019  */
00020
00021
00022 #include<stdio.h>
00023 #include"global.h"
00024
00025 void PrintStress(){
00026   fprintf(fpstress, "%0.4lf\t%0.16lf\t%0.16lf\t%0.16lf\t%0.16lf\n", timeNow, virSumxx, virSumyy,
      virSumxy, pressure);
00027   fflush(fpstress);
00028 }
```

3.80 source/PrintSummary.c File Reference

```
#include <stdio.h>
#include "global.h"
```

Include dependency graph for PrintSummary.c:



Functions

- void PrintSummary ()

3.80.1 Function Documentation

3.80.1.1 PrintSummary()

```
void PrintSummary ( )
```

Definition at line 4 of file PrintSummary.c.

```
00004                   {
00005  fprintf(fpresult, "%0.4lf\t%0.16lf\t%0.16lf\t%0.16lf\t%0.16lf\t%0.16lf\t%0.16lf\t%0.16lf\n",
00006   timeNow, vSum, potEnergy, kinEnergy, totEnergy, uSumPairPerAtom, BondEnergyPerAtom, pressure,
      virSum);
00007   fflush(fpresult);
00008 }
```

References BondEnergyPerAtom, fpresult, kinEnergy, potEnergy, pressure, timeNow, totEnergy, uSumPairPerAtom, virSum, and vSum.

Referenced by main().

Here is the caller graph for this function:

3.81 PrintSummary.c

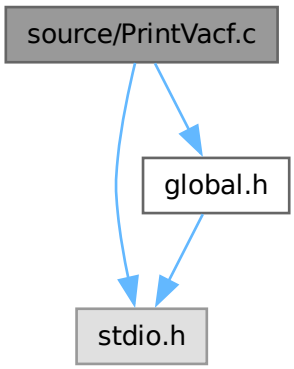
Go to the documentation of this file.

```
00001 #include<stdio.h>
00002 #include"global.h"
00003
00004 void PrintSummary(){
00005  fprintf(fpresult, "%0.4lf\t%0.16lf\t%0.16lf\t%0.16lf\t%0.16lf\t%0.16lf\t%0.16lf\t%0.16lf\t%0.16lf\n",
00006   timeNow, vSum, potEnergy, kinEnergy, totEnergy, uSumPairPerAtom, BondEnergyPerAtom, pressure,
      virSum);
00007   fflush(fpresult);
00008 }
```

3.82 source/PrintVacf.c File Reference

```
#include <stdio.h>
#include "global.h"
```

Include dependency graph for PrintVacf.c:



Functions

- void PrintVacf ()

3.82.1 Function Documentation

3.82.1.1 PrintVacf()

```
void PrintVacf ( )
```

Definition at line 25 of file PrintVacf.c.

```
00025                   {
00026  double tVal;
00027  int j;
00028  fprintf(fpvisc,"viscosity acf\n");
00029  for(j = 1 ; j <= nValAcf ; j ++){
00030   tVal = (j-1)*stepAcf*deltaT;
00031   fprintf(fpvisc, "%lf\t %lf\t %lf\n", tVal, viscAcfAv[j], viscAcfAv[j]/viscAcfAv[1]);
00032   }
00033  fprintf(fpvisc, "viscosity acf integral : %lf\n", viscAcfInt);
00034 }
```

References deltaT, fpvisc, nValAcf, stepAcf, viscAcfAv, and viscAcfInt.

Referenced by AccumVacf().

Here is the caller graph for this function:

3.83 PrintVacf.c

Go to the documentation of this file.

```
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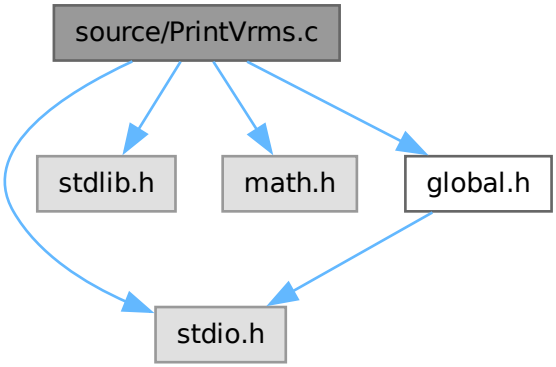
00016
00017  Copyright (C) 2025 Harish Charan, University of Durham, UK
00018
00019  */
00020
00021
00022 #include<stdio.h>
00023 #include"global.h"
```

```
00024
00025 void PrintVacf(){
00026  double tVal;
00027  int j;
00028  fprintf(fpvisc,"viscosity acf\n");
00029  for(j = 1 ; j <= nValAcf ; j ++){
00030   tVal = (j-1)*stepAcf*deltaT;
00031   fprintf(fpvisc, "%lf\t %lf\t %lf\n", tVal, viscAcfAv[j], viscAcfAv[j]/viscAcfAv[1]);
00032   }
00033  fprintf(fpvisc, "viscosity acf integral : %lf\n", viscAcfInt);
00034 }
00035
00036
```

3.84 source/PrintVrms.c File Reference

```
#include <stdio.h>
#include <stdlib.h>
#include <math.h>
#include "global.h"
```

Include dependency graph for PrintVrms.c:



Functions

- void PrintVrms ()

3.84.1 Function Documentation

3.84.1.1 PrintVrms()

```
void PrintVrms ( )
```

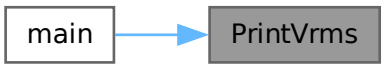
Definition at line 27 of file PrintVrms.c.

```
00027                {
00028  fprintf(fpvrms, "%0.4lf\t%0.16lf\n", timeNow, VRootMeanSqr);
00029  fflush(fpvrms);
00030 }
```

References fpvrms, timeNow, and VRootMeanSqr.

Referenced by main().

Here is the caller graph for this function:



3.85 PrintVrms.c

Go to the documentation of this file.

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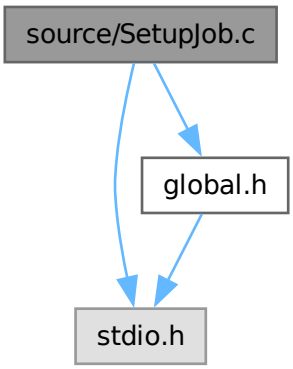
00016
00017  Copyright (C) 2025 Harish Charan, University of Durham, UK
00018
00019  */
00020
00021
00022 #include<stdio.h>
00023 #include<stdlib.h>
00024 #include<math.h>
00025 #include"global.h"
00026
00027 void PrintVrms(){
00028  fprintf(fpvrms, "%0.4lf\t%0.16lf\n", timeNow, VRootMeanSqr);
00029  fflush(fpvrms);
00030 }
00031
00032
00033
```

3.86 source/SetupJob.c File Reference

```
#include <stdio.h>
#include "global.h"
```

Include dependency graph for SetupJob.c:



Functions

- void AllocArrays ()
- void AccumProps (int icode)
- void InitVacf ()
- void SetupJob ()

3.86.1 Function Documentation

3.86.1.1 AccumProps()

```
void AccumProps (
            int icode )
```

Definition at line 25 of file AccumProps.c.

```
00025                           {
00026   if(icode == 0){
00027   sPotEnergy = ssPotEnergy = 0.;
00028   sKinEnergy = ssKinEnergy = 0.;
00029   sPressure = ssPressure = 0.;
00030   sTotEnergy = ssTotEnergy = 0.;
00031   svirSum = 0.;
00032   }else if(icode == 1){
00033   sPotEnergy += potEnergy;
00034   ssPotEnergy += Sqr(potEnergy);
00035   sKinEnergy += kinEnergy;
00036   ssKinEnergy += Sqr(kinEnergy);
00037   sTotEnergy += totEnergy;
00038   ssTotEnergy += Sqr(totEnergy);
00039   sPressure += pressure;
00040   ssPressure += Sqr(pressure);
00041   svirSum += virSum;
00042   }else if(icode == 2){
00043   sPotEnergy /= stepAvg;
00044   ssPotEnergy /= sqrt(ssPotEnergy/stepAvg - Sqr(sPotEnergy));
00045   sTotEnergy /= stepAvg;
00046   ssTotEnergy = sqrt(ssTotEnergy/stepAvg - Sqr(sTotEnergy));
00047   sKinEnergy /= stepAvg;
00048   ssKinEnergy = sqrt(ssKinEnergy/stepAvg - Sqr(sKinEnergy));
00049   sPressure /= stepAvg;
00050   ssPressure = sqrt(ssPressure/stepAvg - Sqr(sPressure));
00051   svirSum /= stepAvg;
```

```
00052   } }
```

References kinEnergy, potEnergy, pressure, sKinEnergy, sPotEnergy, sPressure, Sqr, ssKinEnergy, ssPotEnergy, ssPressure, ssTotEnergy, stepAvg, sTotEnergy, svirSum, totEnergy, and virSum.

Referenced by SetupJob().

Here is the caller graph for this function:

3.86.1.2 AllocArrays()

```
void AllocArrays ( )
```

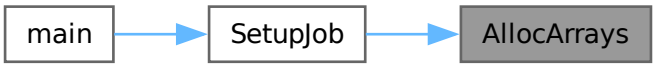
Definition at line 25 of file AllocArrays.c.

```
00025                   {
00026   int n;
00027   // SPACETIME CORRELATIONS
00028   cfOrg = (double **) malloc ((nBuffCorr+1)*sizeof(double *));
00029   for (n = 0; n <= nBuffCorr; n++)
00030    cfOrg[n] = (double *) malloc ((2*nFunCorr+1)*sizeof(double));
00031
00032   cfVal = (double *) malloc ((2*nFunCorr+1)*sizeof(double));
00033   indexCorr = (int *) malloc ((nBuffCorr+1)*sizeof(int));
00034
00035   spacetimeCorr = (double **) malloc ((nBuffCorr+1)*sizeof(double));
00036   for (n = 0; n <= nBuffCorr; n++)
00037   spacetimeCorr[n] = (double *) malloc ((nFunCorr*nValCorr+1)*sizeof(double));
00038
00039   spacetimeCorrAv = (double *) malloc ((nFunCorr*nValCorr+1)*sizeof(double));
00040   // VISCOSITY
00041   indexAcf = (double *)malloc((nBuffAcf+1)*sizeof(double));
00042   viscAcf = (double **)malloc((nBuffAcf+1)*sizeof(double *));
00043   for(n = 0 ; n <= nBuffAcf ; n ++)
00044    viscAcf[n] = (double *)malloc((nValAcf+1)*sizeof(double ));
00045
00046   viscAcfOrg = (double *)malloc((nBuffAcf+1)*sizeof(double));
00047   viscAcfAv = (double *)malloc((nValAcf+1)*sizeof(double));
00048
00049    // RDF
00050    histRdf = (double *)malloc((sizeHistRdf+1)*sizeof(double));
00051 }
```

References cfOrg, cfVal, histRdf, indexAcf, indexCorr, nBuffAcf, nBuffCorr, nFunCorr, nValAcf, nValCorr, sizeHistRdf, spacetimeCorr, spacetimeCorrAv, viscAcf, viscAcfAv, and viscAcfOrg.

Referenced by SetupJob().

Here is the caller graph for this function:



3.86.1.3 InitVacf()

```
void InitVacf ( )
```

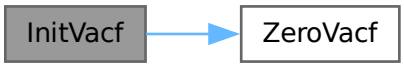
Definition at line 26 of file InitVacf.c.

```
00026                {
00027   int nb;
00028   for(nb = 1 ; nb <= nBuffAcf ; nb ++)
00029     indexAcf[nb] = -(nb-1)*nValAcf/nBuffAcf;
00030   ZeroVacf();
00031 }
```

References indexAcf, nBuffAcf, nValAcf, and ZeroVacf().

Referenced by SetupJob().

Here is the call graph for this function:



Here is the caller graph for this function:

3.86.1.4 SetupJob()

```
void SetupJob ( )
```

Definition at line 27 of file SetupJob.c.

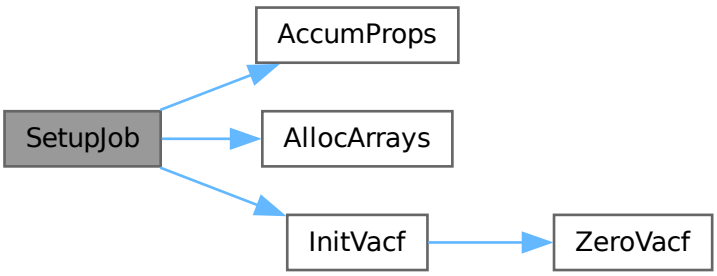
```
00027                {
00028   AllocArrays();
00029   AccumProps(0);
00030   InitVacf();
00031   stepCount = 0;
00032   // INITIALISE SPACETIME CORRELATIONS
00033   int n;
00034   for (n = 1; n <= nBuffCorr; n++)
00035     indexCorr[n] = -(n - 1)*nValCorr/nBuffCorr;
00036
00037   countCorrAv = 0.;
00038
00039   for (n = 1; n <= nFunCorr*nValCorr; n++)
00040     spacetimeCorrAv[n] = 0.;
00041
00042   //RDF
```

```
00043   countRdf = 0;
00044 }
```

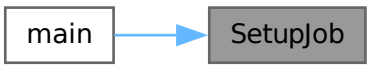
References AccumProps(), AllocArrays(), countCorrAv, countRdf, indexCorr, InitVacf(), nBuffCorr, nFunCorr, nValCorr, spacetimeCorrAv, and stepCount.

Referenced by main().

Here is the call graph for this function:



Here is the caller graph for this function:



3.87 SetupJob.c

Go to the documentation of this file.

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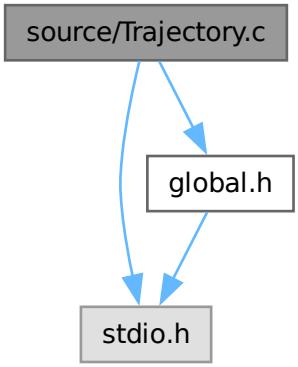
00016
00017  Copyright (C) 2025 Harish Charan, University of Durham, UK
00018
00019  */
```

```
00020
00021 #include<stdio.h>
00022 #include"global.h"
00023
00024 void AllocArrays();
00025 void AccumProps(int icode);
00026 void InitVacf();
00027 void SetupJob(){
00028   AllocArrays();
00029   AccumProps(0);
00030   InitVacf();
00031   stepCount = 0;
00032   // INITIALISE SPACETIME CORRELATIONS
00033   int n;
00034   for (n = 1; n <= nBuffCorr; n++)
00035     indexCorr[n] = -(n - 1)*nValCorr/nBuffCorr;
00036
00037   countCorrAv = 0.;
00038
00039   for (n = 1; n <= nFunCorr*nValCorr; n++)
00040     spacetimeCorrAv[n] = 0.;
00041
00042   //RDF
00043   countRdf = 0;
00044 }
```

3.88 source/Trajectory.c File Reference

```
#include <stdio.h>
#include "global.h"
```

Include dependency graph for Trajectory.c:



Functions

- void Trajectory ()

3.88.1 Function Documentation

3.88.1.1 Trajectory()

```
void Trajectory ( )
```

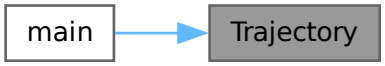
Definition at line 25 of file Trajectory.c.

```
00025                 {
00026  int n;
00027  //Trajectory file in LAMMPS dump format for OVITO visualization
00028  fprintf(fpxyz, "ITEM: TIMESTEP\n");
00029  fprintf(fpxyz, "%lf\n",timeNow);
00030  fprintf(fpxyz, "ITEM: NUMBER OF ATOMS\n");
00031  fprintf(fpxyz, "%d\n",nAtom);
00032  fprintf(fpxyz, "ITEM: BOX BOUNDS pp ff pp\n");
00033  fprintf(fpxyz, "%lf %lf xlo xhi\n", -regionH[1], regionH[1]);
00034  fprintf(fpxyz, "%lf %lf ylo yhi\n", -regionH[2], regionH[2]);
00035  fprintf(fpxyz, "%lf %lf zlo zhi\n", -0.1, 0.1);
00036  fprintf(fpxyz, "ITEM: ATOMS id mol type radius x y vx vy fx fy\n");
00037  for(n=1; n<=nAtom; n++)
00038   fprintf(fpxyz, "%d\t %d\t %d\t %0.2lf\t %0.16lf\t %0.16lf\t %0.16lf\t %0.16lf\t %0.16lf\t
      %0.16lf\n",
00039   atomID[n], molID[n], atomType[n], atomRadius[n], rx[n], ry[n], vx[n], vy[n], ax[n], ay[n]);
00040 }
```

References atomID, atomRadius, atomType, ax, ay, fpxyz, molID, nAtom, regionH, rx, ry, timeNow, vx, and vy.

Referenced by main().

Here is the caller graph for this function:



3.89 Trajectory.c

Go to the documentation of this file.

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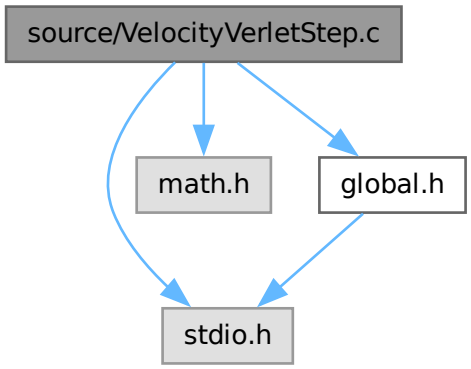
00016
00017  Copyright (C) 2025 Harish Charan, University of Durham, UK
00018
00019  */
00020
00021
00022 #include<stdio.h>
00023 #include"global.h"
00024
00025 void Trajectory(){
00026  int n;
00027  //Trajectory file in LAMMPS dump format for OVITO visualization
00028  fprintf(fpxyz, "ITEM: TIMESTEP\n");
00029  fprintf(fpxyz, "%lf\n",timeNow);
00030  fprintf(fpxyz, "ITEM: NUMBER OF ATOMS\n");
00031  fprintf(fpxyz, "%d\n",nAtom);
00032  fprintf(fpxyz, "ITEM: BOX BOUNDS pp ff pp\n");
00033  fprintf(fpxyz, "%lf %lf xlo xhi\n", -regionH[1], regionH[1]);
00034  fprintf(fpxyz, "%lf %lf ylo yhi\n", -regionH[2], regionH[2]);
00035  fprintf(fpxyz, "%lf %lf zlo zhi\n", -0.1, 0.1);
```

```
00036  fprintf(fpxyz, "ITEM: ATOMS id mol type radius x y vx vy fx fy\n");
00037  for(n=1; n<=nAtom; n++)
00038   fprintf(fpxyz, "%d\t %d\t %d\t %0.2lf\t %0.16lf\t %0.16lf\t %0.16lf\t %0.16lf\t %0.16lf\t
      %0.16lf\n",
00039   atomID[n], molID[n], atomType[n], atomRadius[n], rx[n], ry[n], vx[n], vy[n], ax[n], ay[n]);
00040 }
00041
00042
00043
```

3.90 source/VelocityVerletStep.c File Reference

```
#include <stdio.h>
#include <math.h>
#include "global.h"
```

Include dependency graph for VelocityVerletStep.c:



Functions

- void VelocityVerletStep (int icode)

3.90.1 Function Documentation

3.90.1.1 VelocityVerletStep()

```
void VelocityVerletStep (
            int icode )
```

Definition at line 26 of file VelocityVerletStep.c.

```
00026                                   {
00027 int n;
00028  if(icode == 1){
00029  for (n= 1; n <= nAtom; n++) {
00030   if(atomType[n] != freezeAtomType){
00031   vx[n] += ax[n] * 0.5 * deltaT;
00032   vy[n] += ay[n] * 0.5 * deltaT;
00033   rx[n] += vx[n] * deltaT;
00034   ry[n] += vy[n] * deltaT;
```

```
00035   }
00036   //Calculating the image flags here
00037   if (rx[n] >= regionH[1]) {
00038    rx[n] -= region[1];
00039    ImageX[n]++;
00040    } else if (rx[n] < -regionH[1]) {
00041    rx[n] += region[1];
00042   ImageX[n]--;
00043   }
00044   if (ry[n] >= regionH[2]) {
00045    ry[n] -= region[2];
00046    ImageY[n]++;
00047    } else if (ry[n] < -regionH[2]) {
00048    ry[n] += region[2];
00049    ImageY[n]--;
00050    } } }
00051   else if(icode == 2){
00052   for(n = 1; n <= nAtom; n++) {
00053   if(atomType[n] != freezeAtomType){
00054    vx[n] += ax[n] * 0.5 * deltaT;
00055    vy[n] += ay[n] * 0.5 * deltaT;
00056 } } } }
```

References atomType, ax, ay, deltaT, freezeAtomType, ImageX, ImageY, nAtom, region, regionH, rx, ry, vx, and vy.

Referenced by main().

Here is the caller graph for this function:

3.91 VelocityVerletStep.c

Go to the documentation of this file.

```
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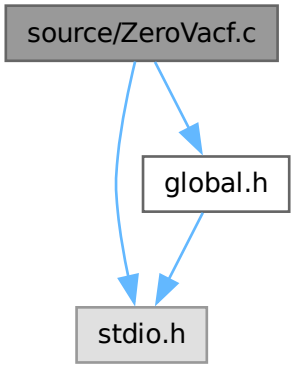
00016
00017  Copyright (C) 2025 Harish Charan, University of Durham, UK
00018
00019  */
00020
00021
00022 #include<stdio.h>
00023 #include<math.h>
00024 #include"global.h"
00025
00026 void VelocityVerletStep(int icode){
00027 int n;
00028  if(icode == 1){
00029  for (n= 1; n <= nAtom; n++) {
```

```
00030   if(atomType[n] != freezeAtomType){
00031   vx[n] += ax[n] * 0.5 * deltaT;
00032   vy[n] += ay[n] * 0.5 * deltaT;
00033   rx[n] += vx[n] * deltaT;
00034   ry[n] += vy[n] * deltaT;
00035   }
00036   //Calculating the image flags here
00037   if (rx[n] >= regionH[1]) {
00038    rx[n] -= region[1];
00039    ImageX[n]++;
00040    } else if (rx[n] < -regionH[1]) {
00041    rx[n] += region[1];
00042   ImageX[n]--;
00043   }
00044   if (ry[n] >= regionH[2]) {
00045    ry[n] -= region[2];
00046    ImageY[n]++;
00047    } else if (ry[n] < -regionH[2]) {
00048    ry[n] += region[2];
00049    ImageY[n]--;
00050    } } }
00051   else if(icode == 2){
00052   for(n = 1; n <= nAtom; n++) {
00053   if(atomType[n] != freezeAtomType){
00054    vx[n] += ax[n] * 0.5 * deltaT;
00055    vy[n] += ay[n] * 0.5 * deltaT;
00056 } } } }
00057
```

3.92 source/ZeroVacf.c File Reference

```
#include <stdio.h>
#include "global.h"
```

Include dependency graph for ZeroVacf.c:



Functions

- void ZeroVacf ()

3.92.1 Function Documentation

3.92.1.1 ZeroVacf()

```
void ZeroVacf ( )
```

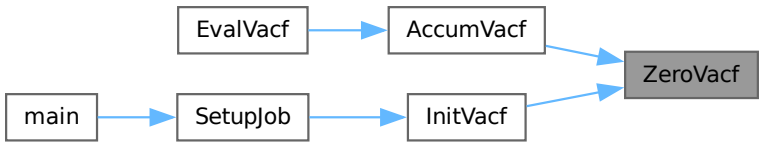
Definition at line 25 of file ZeroVacf.c.

```
00025                {
00026  int j;
00027  countAcfAv= 0 ;
00028  for(j = 1 ; j <= nValAcf ; j ++)
00029   viscAcfAv[j] = 0.;
00030 }
```

References countAcfAv, nValAcf, and viscAcfAv.

Referenced by AccumVacf(), and InitVacf().

Here is the caller graph for this function:



3.93 ZeroVacf.c

Go to the documentation of this file.

```
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00018
00019  */
00020
00021
00022 #include<stdio.h>
00023 #include"global.h"
00024
00025 void ZeroVacf(){
00026  int j;
00027  countAcfAv= 0 ;
00028  for(j = 1 ; j <= nValAcf ; j ++)
00029   viscAcfAv[j] = 0.;
00030 }
```

Index