Lemina

Generated by Doxygen 1.10.0

Chapter 1

Lamina: A Molecular Dynamics Package

Welcome to the **Lamina** documentation!

1.1 Overview

Lamina is a modular 2D molecular dynamics (MD) simulation package designed for simulating hybrid soft solids, including spring networks and finite-size discs. Written in C, it models a wide variety of soft and condensed matter systems. It supports robust time evolution integrators and a range of thermostats, providing accurate force evaluations for bonded and non-bonded interactions.
Originally developed for 2D bonded systems, **Lamina** now supports broader research goals including active matter, granular solids, and complex fluids.

1.2 Why "Lamina"?

The word **Lamina** comes from Latin, meaning "a thin layer", "a plate", or "a sheet". In nature and science, laminae often refer to flat, two-dimensional structural elements such as leaves, thin metal sheets, or tissue membranes.
This name reflects both the **two-dimensional (2D)** nature of the simulations and the types of materials **Lamina** is built to study: **liquids**, **soft solids**, and **networked structures** confined to thin sheets or layers. Just as natural laminae exhibit rich structural and dynamic behaviors in simple geometry, this code explores the complexity of emergent phenomena in 2D soft matter systems.

1.3 Key Features

1.3.1 Interaction Potentials

- Yukawa potential (screened Coulomb interactions)
- Lennard-Jones potential (standard 12-6)
- Harmonic bond potential (elastic network models)
- Hookean granular contact potential (for soft granular matter)

1.3.2 Thermostats and Temperature Control

- Gaussian thermostat
- Nose-Hoover thermostat
- Langevin thermostat
- Configurational temperature evaluation and control

1.3.3 Time Integration

- Leap-Frog integrator
- Velocity-Verlet integrator
- Langevin (stochastic) integrator
- Brownian (overdamped) integrator

1.3.4 Physical Observables

- Radial Distribution Function (RDF)
- Velocity Autocorrelation Function (VACF)
- Root-Mean-Square Velocity (VRMS)
- Stress tensor and momentum
- Center-of-mass motion
- Space-time correlation functions

1.3.5 Output and Utilities

- Output files saved to `../output` folder — ensure this directory exists relative to where you run the code
- Run the simulation with:

```
./main prefix
```

- Structured output files: `.xyz`, `.bond`, `.pair`, `.com`, `.result`
- Restart and resume capability: `.restart` and `.state` files
- Clear separation of source code, unit tests, and output
- Support for Lees–Edwards boundary conditions (sheared systems)
- Configurable halting conditions based on VRMS or custom metrics
- Modular design for easy extension of potentials and features

---

1.4 Project Structure

```
Lamina/
  |-- source/                 # C source files; avoid placing README.md here to prevent extra pages
  |     |-- main.c            # Main driver
  |     |-- *.c, *.h          # Modular source files
  |-- unittest/               # Unit test suite (planned or implemented)
  |     |-- test_*.c          # Individual test cases
  |-- output/                 # Runtime output files
  |-- prepros/                # Preprocessing scripts/tools (.sh, .py, etc.)
  |-- postpros/               # Postprocessing scripts/tools (.sh, .py, etc.)
  |-- doxygen/                # Doxygen configuration and auxiliary files
  |     |-- Doxyfile          # Doxygen config file
  |     |-- header.tex        # Custom LaTeX header for docs
  |     \-- extra_stylesheet.css # Optional CSS for HTML styling
  |-- figures/                # Figures, logos, icons used in docs/code
  |     \-- LogoLaminaLatex.png # Project logo for documentation
  |-- docs/                   # Generated documentation (HTML, LaTeX, PDFs)
  |     |-- html/             # Doxygen-generated HTML docs
  |     |-- latex/            # Doxygen-generated LaTeX sources
  |     \-- refman.pdf        # Generated PDF manual
  |-- Makefile                # Build system for manual Make builds
  |-- CMakeLists.txt          # CMake build system configuration
  |-- README.md               # This main documentation file
  \-- .github/                # GitHub configuration directory
        \-- workflows/        # GitHub Actions workflows for CI/CD
            \-- ci.yml        # CI workflow file
|--generate-docs.sh  #To genrate the html and latex document
```

1.5 Installation Instructions

1.5.1 Prerequisites

1. **GCC Compiler**
   Install `gcc` to compile C code:

   - Ubuntu/Debian:

     ```
     sudo apt-get install build-essential
     ```

   - Fedora/CentOS:

     ```
     sudo dnf install gcc
     ```

   - macOS (via Homebrew):
     `bash brew install gcc`

2. **MPICH (MPI Library)**
   Required for parallel computations:

   - Ubuntu/Debian:

     ```
     sudo apt-get install libmpich-dev
     ```

   - Fedora/CentOS:

     ```
     sudo dnf install mpich
     ```

   - macOS:
     `bash brew install mpich`

3. **CMake (Recommended for modern builds)**
   Install `cmake` to build with the CMake system:

   - Ubuntu/Debian:

     ```
     sudo apt-get install cmake
     ```

   - Fedora/CentOS:

     ```
     sudo dnf install cmake
     ```

   - macOS:
     `bash brew install cmake`

1.6 Building Lamina

You can build Lamina either using the traditional Makefile or the CMake build system.

1.6.1 Using Makefile

```
cd Lamina/source
make clean
make
```

To build and run unit tests:

```
cd ../unittest
make clean
make all
make run
```

1.6.2 Using CMake (Recommended)

This builds the project in a clean isolated directory and manages dependencies automatically.

```
cd Lamina
mkdir -p build
cd build
cmake ..
make -j$(nproc)
```

To run unit tests (assuming they are built in `unittest` and `mpirun` is used):

```
cd ../unittest
make clean
make all
make run
```

1.7 Continuous Integration (CI) with GitHub Actions

The project includes a GitHub Actions workflow (`.github/workflows/ci.yml`) that automates building and testing on Ubuntu runners with MPI installed.
The workflow performs the following:

- Checks out the latest code on push or pull requests to the `main` branch.
- Installs build dependencies including `build-essential`, `cmake`, `mpich`, and MPI development libraries.
- Configures and builds Lamina using CMake in the `build` directory.
- Runs the unit tests in parallel using MPI.

You can view the build status and logs on the **Actions** tab of the GitHub repository.

1.8 Documentation

- Browse full `HTML documentation`
- Download `Source code PDF manual`
- User manual `Physics PDF manual`
- Documentation generated with `Doxygen 1.10.0`

Thank you for your interest in **Lamina**! Contributions and feedback are welcome.
Please check the repository for the latest updates and contact information.

1.9 Adding a Build Status Badge

Chapter 2

File Index

2.1 File List

Here is a list of all files with brief descriptions:

Chapter 3

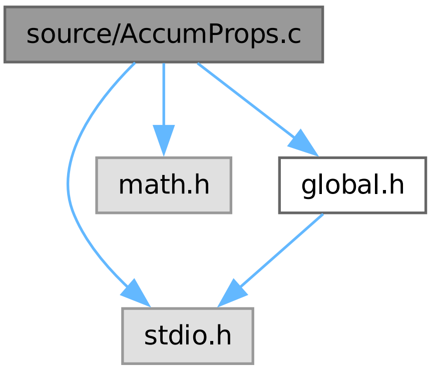
File Documentation

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.

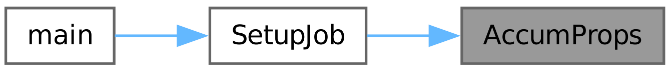
```
                                  {
  if(icode == 0){
  sPotEnergy = ssPotEnergy = 0.;
  sKinEnergy = ssKinEnergy = 0.;
  sPressure = ssPressure = 0.;
```

```
sTotEnergy = ssTotEnergy = 0.;
svirSum = 0.;
}else if(icode == 1){
sPotEnergy += potEnergy;
ssPotEnergy += Sqr(potEnergy);
sKinEnergy += kinEnergy;
ssKinEnergy += Sqr(kinEnergy);
sTotEnergy += totEnergy;
ssTotEnergy += Sqr(totEnergy);
sPressure += pressure;
ssPressure += Sqr(pressure);
svirSum += virSum;
}else if(icode == 2){
sPotEnergy /= stepAvg;
ssPotEnergy /= sqrt(ssPotEnergy/stepAvg - Sqr(sPotEnergy));
sTotEnergy /= stepAvg;
ssTotEnergy = sqrt(ssTotEnergy/stepAvg - Sqr(sTotEnergy));
sKinEnergy /= stepAvg;
ssKinEnergy = sqrt(ssKinEnergy/stepAvg - Sqr(sKinEnergy));
sPressure /= stepAvg;
ssPressure = sqrt(ssPressure/stepAvg - Sqr(sPressure));
svirSum /= stepAvg;
} }
```

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

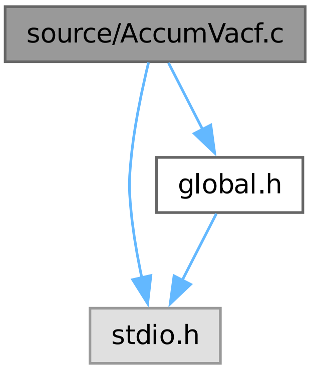
Go to the documentation of this file.

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

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

 */

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

void AccumProps(int icode){
 if(icode == 0){
 sPotEnergy = ssPotEnergy = 0.;
 sKinEnergy = ssKinEnergy = 0.;
 sPressure = ssPressure = 0.;
 sTotEnergy = ssTotEnergy = 0.;
 svirSum = 0.;
 }else if(icode == 1){
 sPotEnergy += potEnergy;
 ssPotEnergy += Sqr(potEnergy);
 sKinEnergy += kinEnergy;
 ssKinEnergy += Sqr(kinEnergy);
 sTotEnergy += totEnergy;
 ssTotEnergy += Sqr(totEnergy);
 sPressure += pressure;
 ssPressure += Sqr(pressure);
 svirSum += virSum;
 }else if(icode == 2){
 sPotEnergy /= stepAvg;
 ssPotEnergy /= sqrt(ssPotEnergy/stepAvg - Sqr(sPotEnergy));
 sTotEnergy /= stepAvg;
 ssTotEnergy = sqrt(ssTotEnergy/stepAvg - Sqr(sTotEnergy));
 sKinEnergy /= stepAvg;
 ssKinEnergy = sqrt(ssKinEnergy/stepAvg - Sqr(sKinEnergy));
 sPressure /= stepAvg;
 ssPressure = sqrt(ssPressure/stepAvg - Sqr(sPressure));
 svirSum /= stepAvg;
 } }
```

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.

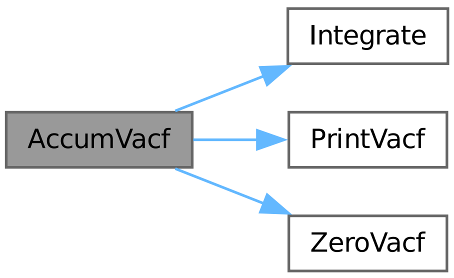
```
                 {
double fac;
int j, nb;
for(nb = 1 ; nb <= nBuffAcf ; nb ++){
 if(indexAcf[nb] == nValAcf){
  for(j = 1 ; j <= nValAcf; j ++){
   viscAcfAv[j] +=  viscAcf[nb][j];
   }
 indexAcf[nb] = 0;
 countAcfAv ++;
```

```
  if(countAcfAv == limitAcfAv){
   fac = 1./(kinEnergy*region[1]*region[2]*limitAcfAv);
   viscAcfInt = fac*stepAcf*deltaT*Integrate(viscAcfAv, nValAcf);
   PrintVacf();
   ZeroVacf();
} } } }
```

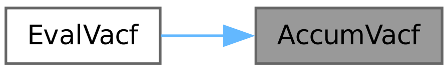
References countAcfAv, deltaT, indexAcf, Integrate(), kinEnergy, limitAcfAv, nBuffAcf, nValAcf, PrintVacf(), region, stepAcf, viscAcf, viscAcfAv, viscAcfInt, and ZeroVacf().

Referenced by EvalVacf().

Here is the call graph for this function:



Here is the caller graph for this function:



3.4.1.2 Integrate()

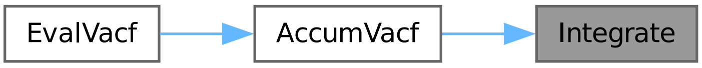
```
double Integrate (
              double * f,
              int nf )
```

Definition at line 25 of file Integrate.c.

```
                                        {
  double s;
  int i;
  s = 0.5*(f[1] + f[nf]);
  for(i = 2 ; i <= nf - 1 ; i ++)
   s += f[i];
  return(s);
}
```

Referenced by AccumVacf().

Here is the caller graph for this function:



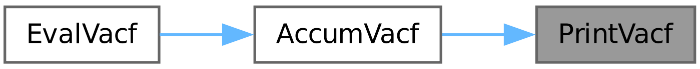
3.4.1.3 PrintVacf()

```
void PrintVacf ( )
```

Definition at line 25 of file PrintVacf.c.

```
                {
 double tVal;
 int j;
 fprintf(fpvisc,"viscosity acf\n");
 for(j = 1 ; j <= nValAcf ; j ++){
  tVal = (j-1)*stepAcf*deltaT;
  fprintf(fpvisc, "%lf\t %lf\t %lf\n", tVal, viscAcfAv[j], viscAcfAv[j]/viscAcfAv[1]);
  }
 fprintf(fpvisc, "viscosity acf integral : %lf\n", viscAcfInt);
}
```

References deltaT, fpvisc, nValAcf, stepAcf, viscAcfAv, and viscAcfInt.
Referenced by AccumVacf().
Here is the caller graph for this function:



3.4.1.4 ZeroVacf()

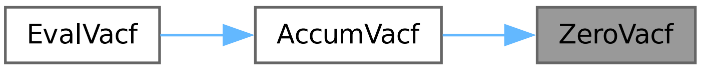
```
void ZeroVacf ( )
```

Definition at line 25 of file ZeroVacf.c.

```
               {
 int j;
 countAcfAv= 0 ;
 for(j = 1 ; j <= nValAcf ; j ++)
  viscAcfAv[j] = 0.;
}
```

References countAcfAv, nValAcf, and viscAcfAv.
Referenced by AccumVacf().

Here is the caller graph for this function:



3.5 AccumVacf.c

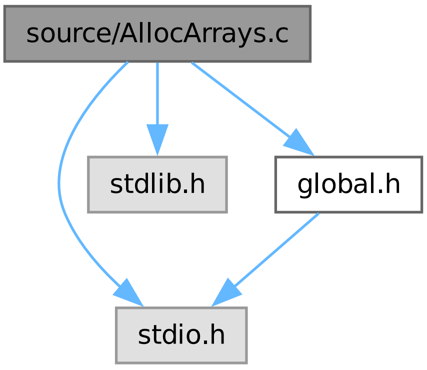
Go to the documentation of this file.

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

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

 */

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

double Integrate(double *, int);
 void PrintVacf();
 void ZeroVacf();
 void AccumVacf(){
 double fac;
 int j, nb;
 for(nb = 1 ; nb <= nBuffAcf ; nb ++){
  if(indexAcf[nb] == nValAcf){
   for(j = 1 ; j <= nValAcf; j ++){
    viscAcfAv[j] +=  viscAcf[nb][j];
    }
  indexAcf[nb] = 0;
  countAcfAv ++;
  if(countAcfAv == limitAcfAv){
   fac = 1./(kinEnergy*region[1]*region[2]*limitAcfAv);
   viscAcfInt = fac*stepAcf*deltaT*Integrate(viscAcfAv, nValAcf);
   PrintVacf();
   ZeroVacf();
} } } }
```

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 ( )
```

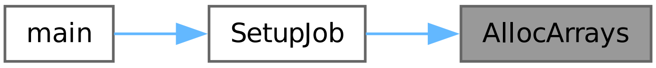
Definition at line 25 of file AllocArrays.c.

```
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.

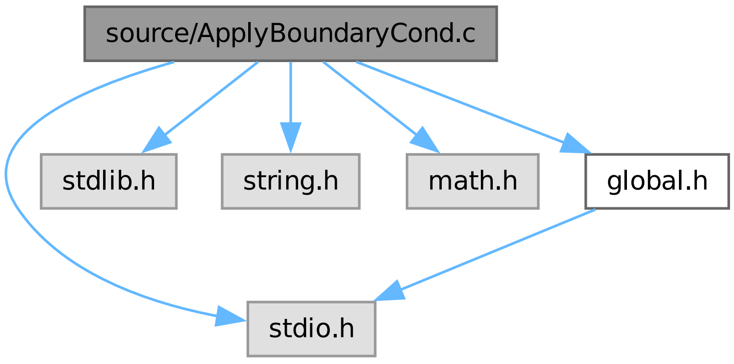
```
/*
 * This file is part of Lamina.
 *
 * Lamina is free software: you can redistribute it and/or modify
 * it under the terms of the GNU General Public License as published by
 * the Free Software Foundation, either version 3 of the License, or
 * (at your option) any later version.
 *
 * Lamina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

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

 */

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

void AllocArrays(){
 int n;
 // SPACETIME CORRELATIONS
 cfOrg = (double **) malloc ((nBuffCorr+1)*sizeof(double *));
 for (n = 0; n <= nBuffCorr; n++)
  cfOrg[n] = (double *) malloc ((2*nFunCorr+1)*sizeof(double));

 cfVal = (double *) malloc ((2*nFunCorr+1)*sizeof(double));
 indexCorr = (int *) malloc ((nBuffCorr+1)*sizeof(int));

 spacetimeCorr = (double **) malloc ((nBuffCorr+1)*sizeof(double));
 for (n = 0; n <= nBuffCorr; n++)
 spacetimeCorr[n] = (double *) malloc ((nFunCorr*nValCorr+1)*sizeof(double));

 spacetimeCorrAv = (double *) malloc ((nFunCorr*nValCorr+1)*sizeof(double));
 // VISCOSITY
 indexAcf = (double *)malloc((nBuffAcf+1)*sizeof(double));
 viscAcf = (double **)malloc((nBuffAcf+1)*sizeof(double *));
 for(n = 0 ; n <= nBuffAcf ; n ++)
  viscAcf[n] = (double *)malloc((nValAcf+1)*sizeof(double ));

 viscAcfOrg = (double *)malloc((nBuffAcf+1)*sizeof(double));
 viscAcfAv = (double *)malloc((nValAcf+1)*sizeof(double));

  // RDF
  histRdf = (double *)malloc((sizeHistRdf+1)*sizeof(double));
}
```

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.

```
                          {
  int n;
  for(n = 1 ; n <= nAtom ; n ++){
   if(strcmp(xBoundary, "p") == 0 && strcmp(yBoundary, "p") == 0){         // P.B.C along x and y axis
    rx[n] -= region[1]*rint(rx[n]/region[1]);
    ry[n] -= region[2]*rint(ry[n]/region[2]);
   } else if (strcmp(xBoundary, "r") == 0 && strcmp(yBoundary, "r") == 0){   //R.B.C. along x and y
axis
     if((rx[n] + atomRadius[n]) >= regionH[1]){
        rx[n] = 0.999999*regionH[1] - atomRadius[n]; vx[n] = -vx[n] ;
     }if((rx[n]-atomRadius[n]) < -regionH[1]){
        rx[n] = -0.999999*regionH[1] + atomRadius[n]; vx[n] = -vx[n] ;
    }
     if((ry[n] + atomRadius[n])>= regionH[2]){
        ry[n] = 0.999999*regionH[2] - atomRadius[n]; vy[n] = -vy[n] ;
     }if((ry[n]-atomRadius[n]) < -regionH[2]){
        ry[n] = -0.999999*regionH[2] + atomRadius[n]; vy[n] = -vy[n] ;
    }}
    else if (strcmp(xBoundary, "p") == 0 && strcmp(yBoundary, "r") == 0){   //P.B.C. along x and R.B.C
along y axis
    rx[n] -= region[1]*rint(rx[n]/region[1]);
    if((ry[n] + atomRadius[n]) >= regionH[2]){
      ry[n] = 0.999999*regionH[2] - atomRadius[n]; vy[n] = -vy[n] ;
     }if((ry[n] - atomRadius[n]) < -regionH[2]){
        ry[n] = -0.999999*regionH[2] + atomRadius[n]; vy[n] = -vy[n] ;
  }}
    else if(strcmp(xBoundary, "r") == 0 && strcmp(yBoundary, "p") == 0){   //R.B.C. along x and P.B.C
along y axis
    if((rx[n] + atomRadius[n]) >= regionH[1]){
       rx[n] = 0.999999*regionH[1] - atomRadius[n]; vx[n] = -vx[n] ;
     }if((rx[n] - atomRadius[n]) < -regionH[1]){
      rx[n] = -0.999999*regionH[1] + atomRadius[n]; vx[n] = -vx[n] ;
     }
     ry[n] -= region[2]*rint(ry[n]/region[2]);
  } else {
    // Print error message and exit the program
    fprintf(fpresult, "Error: Invalid boundary configuration: '%s %s'\n", xBoundary, yBoundary);
    exit(EXIT_FAILURE); // Exit with failure status
  }
 }
}
```

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.

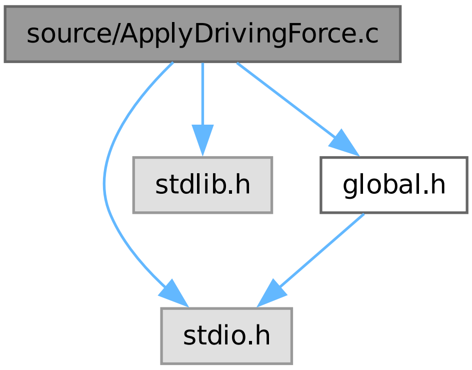
```
/*
 * This file is part of Lamina.
 *
 * Lamina is free software: you can redistribute it and/or modify
 * it under the terms of the GNU General Public License as published by
 * the Free Software Foundation, either version 3 of the License, or
 * (at your option) any later version.
 *
 * Lamina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

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

 */

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

void ApplyBoundaryCond(){
  int n;
  for(n = 1 ; n <= nAtom ; n ++){
   if(strcmp(xBoundary, "p") == 0 && strcmp(yBoundary, "p") == 0){         // P.B.C along x and y axis
    rx[n] -= region[1]*rint(rx[n]/region[1]);
    ry[n] -= region[2]*rint(ry[n]/region[2]);
   } else if (strcmp(xBoundary, "r") == 0 && strcmp(yBoundary, "r") == 0){   //R.B.C. along x and y axis
     if((rx[n] + atomRadius[n]) >= regionH[1]){
        rx[n] = 0.999999*regionH[1] - atomRadius[n]; vx[n] = -vx[n] ;
     }if((rx[n]-atomRadius[n]) < -regionH[1]){
        rx[n] = -0.999999*regionH[1] + atomRadius[n]; vx[n] = -vx[n] ;
    }
     if((ry[n] + atomRadius[n])>= regionH[2]){
        ry[n] = 0.999999*regionH[2] - atomRadius[n]; vy[n] = -vy[n] ;
     }if((ry[n]-atomRadius[n]) < -regionH[2]){
        ry[n] = -0.999999*regionH[2] + atomRadius[n]; vy[n] = -vy[n] ;
    }}
    else if (strcmp(xBoundary, "p") == 0 && strcmp(yBoundary, "r") == 0){   //P.B.C. along x and R.B.C along y axis
    rx[n] -= region[1]*rint(rx[n]/region[1]);
    if((ry[n] + atomRadius[n]) >= regionH[2]){
      ry[n] = 0.999999*regionH[2] - atomRadius[n]; vy[n] = -vy[n] ;
     }if((ry[n] - atomRadius[n]) < -regionH[2]){
        ry[n] = -0.999999*regionH[2] + atomRadius[n]; vy[n] = -vy[n] ;
  }}
    else if(strcmp(xBoundary, "r") == 0 && strcmp(yBoundary, "p") == 0){   //R.B.C. along x and P.B.C along y axis
    if((rx[n] + atomRadius[n]) >= regionH[1]){
       rx[n] = 0.999999*regionH[1] - atomRadius[n]; vx[n] = -vx[n] ;
     }if((rx[n] - atomRadius[n]) < -regionH[1]){
      rx[n] = -0.999999*regionH[1] + atomRadius[n]; vx[n] = -vx[n] ;
     }
```

```
      ry[n] -= region[2]*rint(ry[n]/region[2]);
    } else {
     // Print error message and exit the program
     fprintf(fpresult, "Error: Invalid boundary configuration: '%s %s'\n", xBoundary, yBoundary);
     exit(EXIT_FAILURE); // Exit with failure status
    }
  }
}
```

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.

```
                              {
 int n;
 double Vxblock, Vyblock;
 double Vxsubstrate, Vysubstrate;
 Vxblock = 0.0;  Vyblock = 0.0;
 Vxsubstrate = 0.0; Vysubstrate = 0.0;
 double gammav;
 gammav = 0.0;

 double count_substrate = 0;
 double count_block = 0;

 for(n = 1 ; n <= nAtom; n ++){
  if(atomType[n] == 1 || atomType[n] == 2){
  Vxsubstrate += vx[n]; Vysubstrate += vy[n];
  count_substrate++;
  }
  if(atomType[n] == 3 || atomType[n] == 4){
  Vxblock += vx[n]; Vyblock += vy[n];
  count_block++;
  } }

  if(count_substrate > 0) {
    Vxsubstrate /= count_substrate;
    Vysubstrate /= count_substrate;
  }

  if(count_block > 0) {
   Vxblock /= count_block;
   Vyblock /= count_block;
  }

 for(n = 1 ; n <= nAtom; n ++){
  if(atomType[n] == 1 || atomType[n] == 2){
  ax[n] += -gammav * (vx[n] - Vxsubstrate);
  ay[n] += -gammav * (vy[n] - Vysubstrate);
  }
  if(atomType[n] == 3 || atomType[n] == 4){
  ax[n] += -gammav * (vx[n] - Vxblock);
  ay[n] += -gammav * (vy[n] - Vyblock);
 } } }
```

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

3.11 ApplyDrivingForce.c

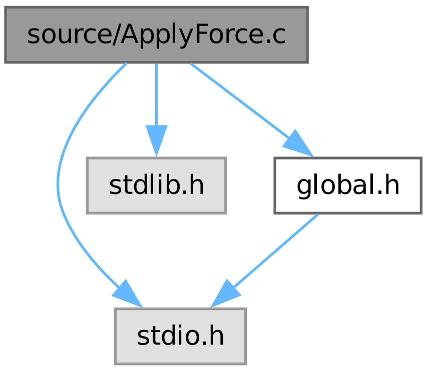
Go to the documentation of this file.

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

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

 */

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

void ApplyDrivingForce(){
 int n;
 double Vxblock, Vyblock;
 double Vxsubstrate, Vysubstrate;
 Vxblock = 0.0;  Vyblock = 0.0;
 Vxsubstrate = 0.0; Vysubstrate = 0.0;
 double gammav;
 gammav = 0.0;

 double count_substrate = 0;
 double count_block = 0;

 for(n = 1 ; n <= nAtom; n ++){
  if(atomType[n] == 1 || atomType[n] == 2){
  Vxsubstrate += vx[n]; Vysubstrate += vy[n];
  count_substrate++;
  }
  if(atomType[n] == 3 || atomType[n] == 4){
  Vxblock += vx[n]; Vyblock += vy[n];
  count_block++;
  } }

  if(count_substrate > 0) {
    Vxsubstrate /= count_substrate;
    Vysubstrate /= count_substrate;
  }

  if(count_block > 0) {
   Vxblock /= count_block;
   Vyblock /= count_block;
  }

 for(n = 1 ; n <= nAtom; n ++){
  if(atomType[n] == 1 || atomType[n] == 2){
  ax[n] += -gammav * (vx[n] - Vxsubstrate);
  ay[n] += -gammav * (vy[n] - Vysubstrate);
  }
  if(atomType[n] == 3 || atomType[n] == 4){
  ax[n] += -gammav * (vx[n] - Vxblock);
  ay[n] += -gammav * (vy[n] - Vyblock);
} } }


```

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 ( )
```

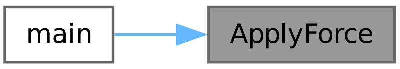
Definition at line 25 of file ApplyForce.c.

```
                    {
int n;
double lx;
lx = regionH[1];
fy =  (FyBylx * lx)/nAtomBlock;
fx =  fxByfy * fy;
for(n = 1; n <= nAtom; n ++){
if(molID[n] == 2){
 ax[n] += fx;
 ay[n] -= fy;
} } }
```

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

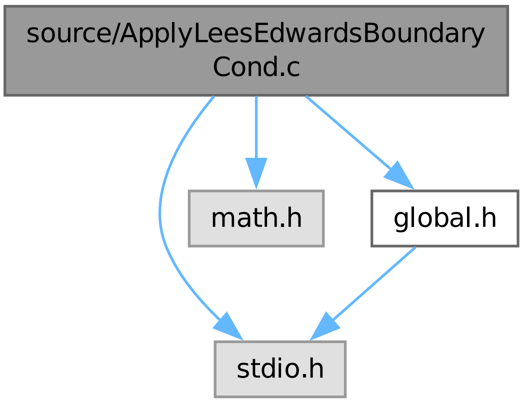
Go to the documentation of this file.

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

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

 */

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

void ApplyForce(){
 int n;
 double lx;
 lx = regionH[1];
 fy =  (FyBylx * lx)/nAtomBlock;
 fx =  fxByfy * fy;
 for(n = 1; n <= nAtom; n ++){
 if(molID[n] == 2){
  ax[n] += fx;
  ay[n] -= fy;
} } }
```

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.

```
                                      {
 int n;
 for (n = 1; n <= nAtom; n++) {
//PBC along x-direction
 if(rx[n] >= regionH[1])
   rx[n] -= region[1];
 else if(rx[n] < -regionH[1])
   rx[n] += region[1];

//LEBC along y-direction
  if(ry[n] >= regionH[2]){
   rx[n] -= shearDisplacement;
   if(rx[n] < -regionH[1]) rx[n] += region[1];
   //vx[n] -= shearVelocity;
   ry[n] -= region[2];
  }else if(ry[n] < -regionH[2]){
   rx[n] += shearDisplacement;
   if(rx[n] >= regionH[1]) rx[n] -= region[1];
   //vx[n] += shearVelocity;
   ry[n] += region[2];
  }
 }
}
```

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

3.15 ApplyLeesEdwardsBoundaryCond.c

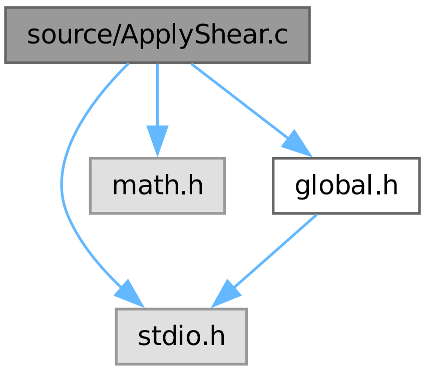
Go to the documentation of this file.

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

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

 */

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

void ApplyLeesEdwardsBoundaryCond() {
 int n;
 for (n = 1; n <= nAtom; n++) {
//PBC along x-direction
 if(rx[n] >= regionH[1])
   rx[n] -= region[1];
 else if(rx[n] < -regionH[1])
   rx[n] += region[1];

//LEBC along y-direction
  if(ry[n] >= regionH[2]){
   rx[n] -= shearDisplacement;
   if(rx[n] < -regionH[1]) rx[n] += region[1];
   //vx[n] -= shearVelocity;
   ry[n] -= region[2];
  }else if(ry[n] < -regionH[2]){
   rx[n] += shearDisplacement;
   if(rx[n] >= regionH[1]) rx[n] -= region[1];
   //vx[n] += shearVelocity;
   ry[n] += region[2];
  }
 }
}
```

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.

```
                    {
 int n;
 for(n = 1 ; n <= nAtom ; n ++){
  rx[n] += strain * ry[n];
  //vx[n] += stranRate * ry[n];
 } }
```

References nAtom, rx, ry, and strain.

3.17 ApplyShear.c

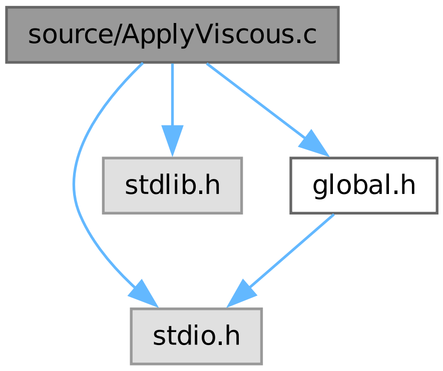
Go to the documentation of this file.

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

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

 */

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

void ApplyShear(){
 int n;
 for(n = 1 ; n <= nAtom ; n ++){
  rx[n] += strain * ry[n];
  //vx[n] += stranRate * ry[n];
 } }
```

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

Go to the documentation of this file.

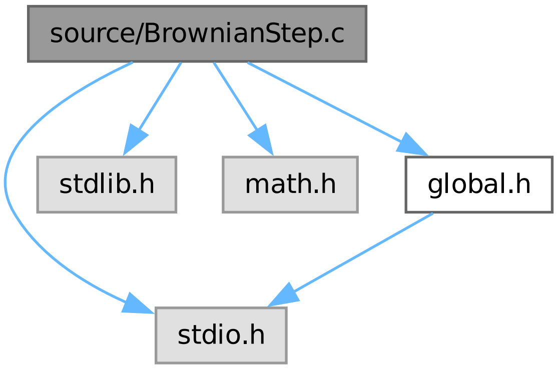
```
00001 /*
00002  * This file is part of Lamina.
00003  *
00004  * Lamina is free software: you can redistribute it and/or modify
00005  * it under the terms of the GNU General Public License as published by
00006  * the Free Software Foundation, either version 3 of the License, or
00007  * (at your 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
```

```
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++){
      vx[n] = C * vx[n] + D * ax[n];
      rx[n] += deltaT * vx[n];
      vy[n] = C * vy[n] + D * ay[n];
      ry[n] += deltaT * vy[n];
    }
  }else{
      int n;
      //SETTING TEMP = 0.0
     if (stepCount == stepEquil+1){
     for(n = 1 ; n <= nAtom ; n ++){
     vx[n] = 0.0;
     vy[n] = 0.0;
     }}
     double zeta = 1.0;
     double dx, dy;
     for(n = 1 ; n <= nAtom ; n ++){
      dx = rx[n];
      rx[n] += zeta * ax[n] * deltaT;
      dx = rx[n] - dx;
      vx[n] = dx/deltaT;
      dy = ry[n];
      ry[n] += zeta * ay[n] * deltaT;
      dy = ry[n] - dy;
      vy[n] = dy/deltaT;
    }
  }
}
```

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

3.21 BrownianStep.c

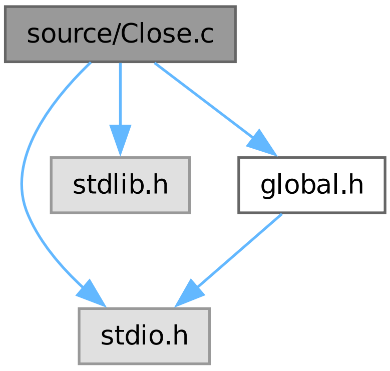
Go to the documentation of this file.

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

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

 */

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

void BrownianStep(){
  if(stepCount <= stepEquil){
    double A, S1, S2, T;
    int n;
    S1 = 0.; S2 = 0;
    double halfdt = 0.5*deltaT;
    for (n = 1; n <= nAtom; n++){
      T = vx[n] + halfdt * ax[n];
      S1 += T * ax[n];
      S2 += Sqr(T);

      T = vy[n] + halfdt * ay[n];
      S1 += T * ay[n];
      S2 += Sqr(T);
    }
    A = -S1 / S2;
    double C = 1 + A*deltaT ;
    double D = deltaT * (1 + 0.5 * A * deltaT);
    for (n = 1; n <= nAtom; n++){
      vx[n] = C * vx[n] + D * ax[n];
      rx[n] += deltaT * vx[n];
      vy[n] = C * vy[n] + D * ay[n];
      ry[n] += deltaT * vy[n];
    }
  }else{
      int n;
      //SETTING TEMP = 0.0
     if (stepCount == stepEquil+1){
     for(n = 1 ; n <= nAtom ; n ++){
     vx[n] = 0.0;
     vy[n] = 0.0;
     }}
     double zeta = 1.0;
     double dx, dy;
     for(n = 1 ; n <= nAtom ; n ++){
      dx = rx[n];
      rx[n] += zeta * ax[n] * deltaT;
      dx = rx[n] - dx;
      vx[n] = dx/deltaT;
      dy = ry[n];
      ry[n] += zeta * ay[n] * deltaT;
      dy = ry[n] - dy;
      vy[n] = dy/deltaT;
    }
  }
}
```

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 ( )
```

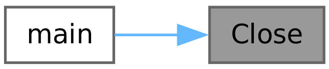
Definition at line 24 of file Close.c.

```
                {
  int n;
  free(rx);
  free(ry);
  free(vx);
  free(vy);
  free(ax);
  free(ay);
  free(fax);
  free(fay);
  free(cellList);

  free(atomID); free(atomType); free(atomRadius); free(atomMass);
  free(speed);
  free(atom1); free(atom2); free(BondID);
  free(BondType); free(kb); free(ro);
  free(ImageX); free(ImageY); free(rxUnwrap); free(ryUnwrap);
  free(atomIDInterface);
  free(PairID); free(Pairatom1); free(Pairatom2);
  free(PairXij); free(PairYij);

  free(DeltaXijOld);
  free(DeltaYijOld);

  free(molID);

  for (n = 0; n <= nAtom; n++) {
   free(isBonded[n]);
   }
   free(isBonded);



  for(n = 0; n <= nAtom; n++) {
   free(DeltaXijOldPair[n]);
   free(DeltaYijOldPair[n]);
   }
    free(DeltaXijOldPair);
    free(DeltaYijOldPair);

  for (n = 0; n <= nBuffCorr; n++){
    free(cfOrg[n]);
    free(spacetimeCorr[n]);
  }
  free(cfOrg);
  free(spacetimeCorr);
  free(cfVal);
  free(indexCorr);
  free(spacetimeCorrAv);

  free(indexAcf);
  free(viscAcfOrg);
  free(viscAcfAv);
  for(n = 0 ; n <= nBuffAcf ; n ++)
    free(viscAcf[n]);
  free(viscAcf);

}
```

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.

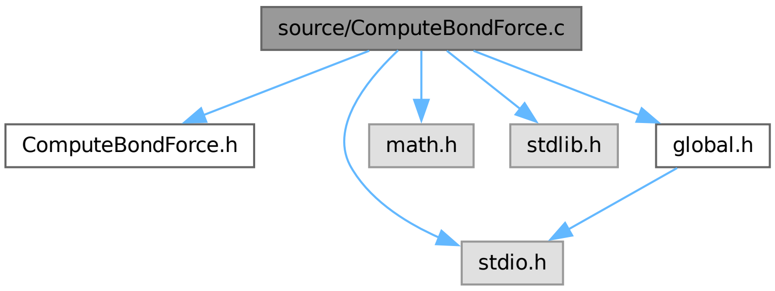
```
/*
 * This file is part of Lamina.
 *
 * Lamina is free software: you can redistribute it and/or modify
 * it under the terms of the GNU General Public License as published by
 * the Free Software Foundation, either version 3 of the License, or
 * (at your option) any later version.
 *
 * Lamina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

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

 */

#include<stdio.h>
#include<stdlib.h>
#include"global.h"
void Close(){
  int n;
  free(rx);
  free(ry);
  free(vx);
  free(vy);
  free(ax);
  free(ay);
  free(fax);
  free(fay);
  free(cellList);

  free(atomID); free(atomType); free(atomRadius); free(atomMass);
  free(speed);
  free(atom1); free(atom2); free(BondID);
  free(BondType); free(kb); free(ro);
  free(ImageX); free(ImageY); free(rxUnwrap); free(ryUnwrap);
  free(atomIDInterface);
  free(PairID); free(Pairatom1); free(Pairatom2);
  free(PairXij); free(PairYij);

  free(DeltaXijOld);
  free(DeltaYijOld);

  free(molID);

  for (n = 0; n <= nAtom; n++) {
   free(isBonded[n]);
   }
   free(isBonded);



  for(n = 0; n <= nAtom; n++) {
   free(DeltaXijOldPair[n]);
   free(DeltaYijOldPair[n]);
   }
    free(DeltaXijOldPair);
    free(DeltaYijOldPair);

  for (n = 0; n <= nBuffCorr; n++){
    free(cfOrg[n]);
    free(spacetimeCorr[n]);
  }
  free(cfOrg);
  free(spacetimeCorr);
  free(cfVal);
  free(indexCorr);
  free(spacetimeCorrAv);

  free(indexAcf);
  free(viscAcfOrg);
  free(viscAcfAv);
  for(n = 0 ; n <= nBuffAcf ; n ++)
    free(viscAcf[n]);
  free(viscAcf);

}
```

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.

```
                              {
  int n;
  double dr[NDIM+1], r, rr, ri, roi;
  double uVal, fcVal;

  uVal = 0.0; TotalBondEnergy = 0.0;
  virSumBond = 0.0; virSumBondxx = 0.0; virSumBondyy = 0.0; virSumBondxy = 0.0;

  double vr[NDIM+1], fdVal, rri;

  for(n = 1 ; n <= nAtom ; n ++){
   nodeDragx[n] = 0.0;
   nodeDragy[n] = 0.0;
  } //Important change made on 03Apr2025. Mention it in GitHub

  int atom1ID, atom2ID;

  for(n=1; n<=nBond; n++){
   rr = 0.0; rri = 0.0; fcVal = 0.0;  fdVal = 0.0; strech = 0.0;
   atom1ID = atom1[n];
   atom2ID = atom2[n];

   dr[1] = rx[atom1ID] - rx[atom2ID];
   if(dr[1] >= regionH[1])
    dr[1] -= region[1];
   else if(dr[1] < -regionH[1])
    dr[1] += region[1];

   dr[2] = ry[atom1ID] - ry[atom2ID];
   if(dr[2] >= regionH[2]){
    dr[1] -= shearDisplacement;
    if(dr[1] < -regionH[1]) dr[1] += region[1];
    dr[2] -= region[2];
  }else if(dr[2] < -regionH[2]){
   dr[1] += shearDisplacement;
    if(dr[1] >= regionH[1]) dr[1] -= region[1];
   dr[2] += region[2];
  }

   rr = Sqr(dr[1]) + Sqr(dr[2]);
   r = sqrt(rr);
   rri = 1.0/rr;
   ri = 1.0/r;
   roi = 1.0/ro[n];
   strech = (r * roi - 1.0);
   uVal = 0.5 * kb[n] * ro[n] * Sqr(strech);
   fcVal = -kb[n] * strech * ri; //F = -Grad U

   vr[1] = vx[atom1ID] - vx[atom2ID];
   vr[2] = vy[atom1ID] - vy[atom2ID];
   fdVal = -gamman * (vr[1]*dr[1] + vr[2]*dr[2]) * rri; //node-node drag

   //DampFlag = 1. LAMMPS version
   if(DampFlag == 1){
   nodeDragx[atom1ID] =  fdVal * dr[1];  //node-node drag  //Important change made on 03Apr2025. Mention it in GitHub
   nodeDragy[atom1ID] =  fdVal * dr[2];  //node-node drag  //Adding the drag forces is wrong. Only add the
   nodeDragx[atom2ID] =  -fdVal * dr[1];  //node-node drag //total force
   nodeDragy[atom2ID] =  -fdVal * dr[2];  //node-node drag

   ax[atom1ID] +=  (fcVal + fdVal) * dr[1];
   ay[atom1ID] +=  (fcVal + fdVal) * dr[2];
   ax[atom2ID] += -(fcVal + fdVal) * dr[1];
   ay[atom2ID] += -(fcVal + fdVal) * dr[2];
   }

   //DampFlag = 2. Suzanne notes version
   else if(DampFlag == 2){
   nodeDragx[atom1ID] =  -gamman * vr[1];  //node-node drag
   nodeDragy[atom1ID] =  -gamman * vr[2]; //node-node drag
   nodeDragx[atom2ID] =  -(-gamman * vr[1]);  //node-node drag
   nodeDragy[atom2ID] =  -(-gamman * vr[2]);  //node-node drag

   ax[atom1ID] +=  (fcVal * dr[1] - gamman * vr[1]);
   ay[atom1ID] +=  (fcVal * dr[2] - gamman * vr[2]);
   ax[atom2ID] += -(fcVal * dr[1] - gamman * vr[1]);
   ay[atom2ID] += -(fcVal * dr[2] - gamman * vr[2]);
   }

   //DampFlag = 3. Suzanne PRL, 130, 178203 (2023) version
   else if(DampFlag == 3){
    DeltaXijNew = dr[1];
    DeltaYijNew = dr[2];

    if(stepCount == 0) {  // First timestep
     DeltaXijOld[n] = DeltaXijNew;
     DeltaYijOld[n] = DeltaYijNew;
    }

    DeltaXij = DeltaXijNew - DeltaXijOld[n];
    DeltaYij = DeltaYijNew - DeltaYijOld[n];
    DeltaVXij = DeltaXij / deltaT;
    DeltaVYij = DeltaYij / deltaT;

    // Now update for the next timestep
    DeltaXijOld[n] = DeltaXijNew;
    DeltaYijOld[n] = DeltaYijNew;

    nodeDragx[atom1ID] =  -gamman * DeltaVXij;  //node-node drag
    nodeDragy[atom1ID] =  -gamman * DeltaVYij; //node-node drag
    nodeDragx[atom2ID] =  -(-gamman * DeltaVXij);  //node-node drag
    nodeDragy[atom2ID] =  -(-gamman * DeltaVYij);  //node-node drag

    ax[atom1ID] +=  (fcVal * dr[1] - gamman * DeltaVXij);
    ay[atom1ID] +=  (fcVal * dr[2] - gamman * DeltaVYij);
    ax[atom2ID] += -(fcVal * dr[1] - gamman * DeltaVXij);
    ay[atom2ID] += -(fcVal * dr[2] - gamman * DeltaVYij);
   }


   BondLength[n] = r;
   BondEnergy[n] = uVal; //No 0.5 factor since it is the energy of the bond
   TotalBondEnergy   +=  BondEnergy[n];

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

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:

main
ComputeBondForce

3.25 ComputeBondForce.c

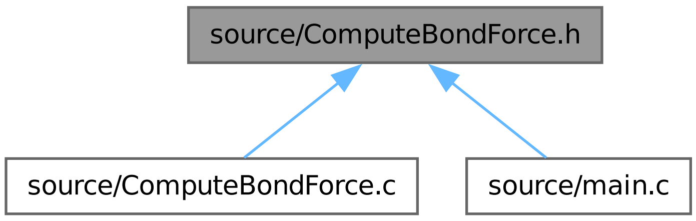
Go to the documentation of this file.

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

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

 */

#include "ComputeBondForce.h"

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

void ComputeBondForce(){
  int n;
  double dr[NDIM+1], r, rr, ri, roi;
  double uVal, fcVal;

  uVal = 0.0; TotalBondEnergy = 0.0;
  virSumBond = 0.0; virSumBondxx = 0.0; virSumBondyy = 0.0; virSumBondxy = 0.0;

  double vr[NDIM+1], fdVal, rri;

  for(n = 1 ; n <= nAtom ; n ++){
   nodeDragx[n] = 0.0;
   nodeDragy[n] = 0.0;
  } //Important change made on 03Apr2025. Mention it in GitHub

  int atom1ID, atom2ID;

  for(n=1; n<=nBond; n++){
   rr = 0.0; rri = 0.0; fcVal = 0.0;  fdVal = 0.0; strech = 0.0;
   atom1ID = atom1[n];
   atom2ID = atom2[n];

   dr[1] = rx[atom1ID] - rx[atom2ID];
   if(dr[1] >= regionH[1])
    dr[1] -= region[1];
   else if(dr[1] < -regionH[1])
    dr[1] += region[1];

   dr[2] = ry[atom1ID] - ry[atom2ID];
   if(dr[2] >= regionH[2]){
    dr[1] -= shearDisplacement;
    if(dr[1] < -regionH[1]) dr[1] += region[1];
    dr[2] -= region[2];
  }else if(dr[2] < -regionH[2]){
   dr[1] += shearDisplacement;
    if(dr[1] >= regionH[1]) dr[1] -= region[1];
```

```c
   dr[2] += region[2];
  }

   rr = Sqr(dr[1]) + Sqr(dr[2]);
   r = sqrt(rr);
   rri = 1.0/rr;
   ri = 1.0/r;
   roi = 1.0/ro[n];
   strech = (r * roi - 1.0);
   uVal = 0.5 * kb[n] * ro[n] * Sqr(strech);
   fcVal = -kb[n] * strech * ri; //F = -Grad U

   vr[1] = vx[atom1ID] - vx[atom2ID];
   vr[2] = vy[atom1ID] - vy[atom2ID];
   fdVal = -gamman * (vr[1]*dr[1] + vr[2]*dr[2]) * rri; //node-node drag

   //DampFlag = 1. LAMMPS version
   if(DampFlag == 1){
   nodeDragx[atom1ID] =  fdVal * dr[1];  //node-node drag  //Important change made on 03Apr2025. Mention it in GitHub
   nodeDragy[atom1ID] =  fdVal * dr[2];  //node-node drag  //Adding the drag forces is wrong. Only add the
   nodeDragx[atom2ID] =  -fdVal * dr[1];  //node-node drag //total force
   nodeDragy[atom2ID] =  -fdVal * dr[2];  //node-node drag

   ax[atom1ID] +=  (fcVal + fdVal) * dr[1];
   ay[atom1ID] +=  (fcVal + fdVal) * dr[2];
   ax[atom2ID] += -(fcVal + fdVal) * dr[1];
   ay[atom2ID] += -(fcVal + fdVal) * dr[2];
   }

   //DampFlag = 2. Suzanne notes version
   else if(DampFlag == 2){
   nodeDragx[atom1ID] =  -gamman * vr[1];  //node-node drag
   nodeDragy[atom1ID] =  -gamman * vr[2]; //node-node drag
   nodeDragx[atom2ID] =  -(-gamman * vr[1]);  //node-node drag
   nodeDragy[atom2ID] =  -(-gamman * vr[2]);  //node-node drag

   ax[atom1ID] +=  (fcVal * dr[1] - gamman * vr[1]);
   ay[atom1ID] +=  (fcVal * dr[2] - gamman * vr[2]);
   ax[atom2ID] += -(fcVal * dr[1] - gamman * vr[1]);
   ay[atom2ID] += -(fcVal * dr[2] - gamman * vr[2]);
   }

   //DampFlag = 3. Suzanne PRL, 130, 178203 (2023) version
   else if(DampFlag == 3){
    DeltaXijNew = dr[1];
    DeltaYijNew = dr[2];

    if(stepCount == 0) {  // First timestep
     DeltaXijOld[n] = DeltaXijNew;
     DeltaYijOld[n] = DeltaYijNew;
    }

    DeltaXij = DeltaXijNew - DeltaXijOld[n];
    DeltaYij = DeltaYijNew - DeltaYijOld[n];
    DeltaVXij = DeltaXij / deltaT;
    DeltaVYij = DeltaYij / deltaT;

    // Now update for the next timestep
    DeltaXijOld[n] = DeltaXijNew;
    DeltaYijOld[n] = DeltaYijNew;

    nodeDragx[atom1ID] =  -gamman * DeltaVXij;  //node-node drag
    nodeDragy[atom1ID] =  -gamman * DeltaVYij; //node-node drag
    nodeDragx[atom2ID] =  -(-gamman * DeltaVXij);  //node-node drag
    nodeDragy[atom2ID] =  -(-gamman * DeltaVYij);  //node-node drag

    ax[atom1ID] +=  (fcVal * dr[1] - gamman * DeltaVXij);
    ay[atom1ID] +=  (fcVal * dr[2] - gamman * DeltaVYij);
    ax[atom2ID] += -(fcVal * dr[1] - gamman * DeltaVXij);
    ay[atom2ID] += -(fcVal * dr[2] - gamman * DeltaVYij);
   }


   BondLength[n] = r;
   BondEnergy[n] = uVal; //No 0.5 factor since it is the energy of the bond
   TotalBondEnergy   +=  BondEnergy[n];

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

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 ( )
```

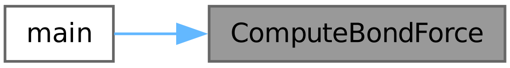
Definition at line 28 of file ComputeBondForce.c.

```
                             {
  int n;
  double dr[NDIM+1], r, rr, ri, roi;
  double uVal, fcVal;

  uVal = 0.0; TotalBondEnergy = 0.0;
  virSumBond = 0.0; virSumBondxx = 0.0; virSumBondyy = 0.0; virSumBondxy = 0.0;

  double vr[NDIM+1], fdVal, rri;

  for(n = 1 ; n <= nAtom ; n ++){
   nodeDragx[n] = 0.0;
   nodeDragy[n] = 0.0;
  } //Important change made on 03Apr2025. Mention it in GitHub

  int atom1ID, atom2ID;

  for(n=1; n<=nBond; n++){
   rr = 0.0; rri = 0.0; fcVal = 0.0;  fdVal = 0.0; strech = 0.0;
   atom1ID = atom1[n];
   atom2ID = atom2[n];

   dr[1] = rx[atom1ID] - rx[atom2ID];
   if(dr[1] >= regionH[1])
    dr[1] -= region[1];
   else if(dr[1] < -regionH[1])
    dr[1] += region[1];

   dr[2] = ry[atom1ID] - ry[atom2ID];
   if(dr[2] >= regionH[2]){
    dr[1] -= shearDisplacement;
    if(dr[1] < -regionH[1]) dr[1] += region[1];
    dr[2] -= region[2];
  }else if(dr[2] < -regionH[2]){
   dr[1] += shearDisplacement;
    if(dr[1] >= regionH[1]) dr[1] -= region[1];
   dr[2] += region[2];
  }

   rr = Sqr(dr[1]) + Sqr(dr[2]);
   r = sqrt(rr);
   rri = 1.0/rr;
   ri = 1.0/r;
   roi = 1.0/ro[n];
   strech = (r * roi - 1.0);
   uVal = 0.5 * kb[n] * ro[n] * Sqr(strech);
   fcVal = -kb[n] * strech * ri; //F = -Grad U

   vr[1] = vx[atom1ID] - vx[atom2ID];
   vr[2] = vy[atom1ID] - vy[atom2ID];
   fdVal = -gamman * (vr[1]*dr[1] + vr[2]*dr[2]) * rri; //node-node drag

   //DampFlag = 1. LAMMPS version
   if(DampFlag == 1){
   nodeDragx[atom1ID] =  fdVal * dr[1];  //node-node drag  //Important change made on 03Apr2025. Mention it in GitHub
   nodeDragy[atom1ID] =  fdVal * dr[2];  //node-node drag  //Adding the drag forces is wrong. Only add the
   nodeDragx[atom2ID] =  -fdVal * dr[1];  //node-node drag //total force
   nodeDragy[atom2ID] =  -fdVal * dr[2];  //node-node drag

   ax[atom1ID] +=  (fcVal + fdVal) * dr[1];
   ay[atom1ID] +=  (fcVal + fdVal) * dr[2];
   ax[atom2ID] += -(fcVal + fdVal) * dr[1];
   ay[atom2ID] += -(fcVal + fdVal) * dr[2];
   }

   //DampFlag = 2. Suzanne notes version
   else if(DampFlag == 2){
   nodeDragx[atom1ID] =  -gamman * vr[1];  //node-node drag
   nodeDragy[atom1ID] =  -gamman * vr[2]; //node-node drag
   nodeDragx[atom2ID] =  -(-gamman * vr[1]);  //node-node drag
   nodeDragy[atom2ID] =  -(-gamman * vr[2]);  //node-node drag

   ax[atom1ID] +=  (fcVal * dr[1] - gamman * vr[1]);
   ay[atom1ID] +=  (fcVal * dr[2] - gamman * vr[2]);
   ax[atom2ID] += -(fcVal * dr[1] - gamman * vr[1]);
   ay[atom2ID] += -(fcVal * dr[2] - gamman * vr[2]);
   }

   //DampFlag = 3. Suzanne PRL, 130, 178203 (2023) version
   else if(DampFlag == 3){
    DeltaXijNew = dr[1];
    DeltaYijNew = dr[2];

    if(stepCount == 0) {  // First timestep
     DeltaXijOld[n] = DeltaXijNew;
     DeltaYijOld[n] = DeltaYijNew;
    }

    DeltaXij = DeltaXijNew - DeltaXijOld[n];
    DeltaYij = DeltaYijNew - DeltaYijOld[n];
    DeltaVXij = DeltaXij / deltaT;
    DeltaVYij = DeltaYij / deltaT;

    // Now update for the next timestep
    DeltaXijOld[n] = DeltaXijNew;
    DeltaYijOld[n] = DeltaYijNew;

    nodeDragx[atom1ID] =  -gamman * DeltaVXij;  //node-node drag
    nodeDragy[atom1ID] =  -gamman * DeltaVYij; //node-node drag
    nodeDragx[atom2ID] =  -(-gamman * DeltaVXij);  //node-node drag
    nodeDragy[atom2ID] =  -(-gamman * DeltaVYij);  //node-node drag

    ax[atom1ID] +=  (fcVal * dr[1] - gamman * DeltaVXij);
    ay[atom1ID] +=  (fcVal * dr[2] - gamman * DeltaVYij);
    ax[atom2ID] += -(fcVal * dr[1] - gamman * DeltaVXij);
    ay[atom2ID] += -(fcVal * dr[2] - gamman * DeltaVYij);
   }


   BondLength[n] = r;
   BondEnergy[n] = uVal; //No 0.5 factor since it is the energy of the bond
   TotalBondEnergy   +=  BondEnergy[n];

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

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

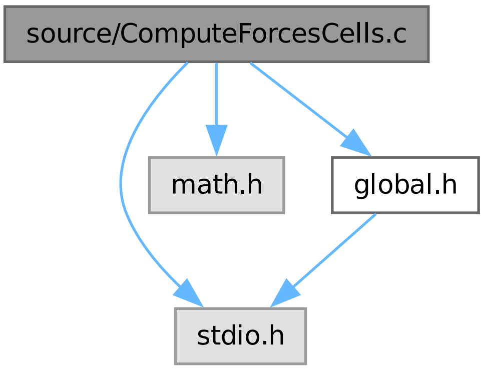
Go to the documentation of this file.

```
#ifndef COMPUTE_BOND_FORCE_H
#define COMPUTE_BOND_FORCE_H

void ComputeBondForce();

#endif

```

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
```

```
        uSum +=  0.5 * uVal;
        virSum += 0.5 * fcVal * rr;
        rfAtom += 0.5 * dr[1] * fcVal * dr[2];
          }
        }else if(m1 != m2 && (atomRadius[I] > 0. && atomRadius[J] > 0.)){
          dr[1] = rx[I] - rx[J] - shift[1];
          dr[2] = ry[I] - ry[J] - shift[2];
          rr = Sqr(dr[1]) + Sqr(dr[2]);
          RadiusIJ = atomRadius[I] + atomRadius[J];
          SqrRadiusIJ = Sqr(RadiusIJ);
          if(rr < SqrRadiusIJ){
        r = sqrt(rr);
        ri = 1.0/r;
                rrinv = 1.0/r;
                vr[1] = vx[I] - vx[J];
                vr[2] = vy[I] - vy[J];
        RadiusIJInv = 1.0/RadiusIJ;
        uVal = Sqr(1.0 - r * RadiusIJInv);
        fcVal = 2.0 * RadiusIJInv * (1.0 - r * RadiusIJInv) *ri;
                fdVal = -gamman * (vr[1]*dr[1] + vr[2]*dr[2]) * rrinv; //disc-disc drag

        f  = fcVal * dr[1];
                fd =  fdVal * dr[1];
        ax[I] += (f + fd);
                discDragx[I] += fd; //disc-disc drag

        f  = fcVal * dr[2];
                fd = fdVal * dr[2];
        ay[I] += (f + fd);
                discDragy[I] += fd; //disc-disc drag

        uSum +=  0.5 * uVal;
        virSum += 0.5 * fcVal * rr;
        rfAtom += 0.5 * dr[1] * fcVal * dr[2];
          }
        }
            J = cellList[J];
      }
      I = cellList[I];
    }
      }
    }
  }
}
```

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

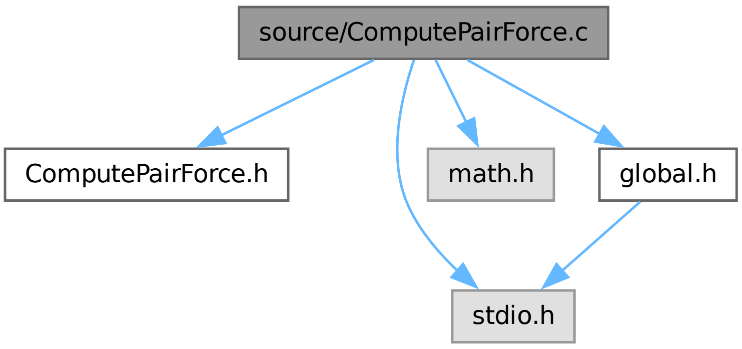
Go to the documentation of this file.

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

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

 */

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

void ComputeForcesCells(){
  double dr[NDIM+1], invWid[NDIM+1], shift[NDIM+1], f, fcVal, rr, ri, r, uVal;
  int c, I, J, m1, m1X, m1Y, m2, m2X, m2Y, n, offset;
  int iofX[] = {0, 0, 1, 1, 0, -1, -1, -1, 0, 1},
      iofY[] = {0, 0, 0, 1 ,1, 1, 0, -1, -1, -1};

  invWid[1] = cells[1]/region[1];
  invWid[2] = cells[2]/region[2];

  for(n = nAtom+1; n <= nAtom+cells[1]*cells[2] ; n++)
    cellList[n] = 0;

  for(n = 1 ; n <= nAtom ; n ++){
    c = ((int)((ry[n] + regionH[2])*invWid[2]))*cells[1] + (int)((rx[n]+regionH[1])*invWid[1]) +
nAtom+ 1;
    cellList[n] = cellList[c];
    cellList[c] = n;
  }

  for(n = 1 ; n <= nAtom ; n ++){
    ax[n] = 0.;
    ay[n] = 0.;
  }

  uSum = 0.0 ;
  virSum = 0.0;
  rfAtom = 0.0;
  RadiusIJ = 0.0;

  gamman = 1.0;
  double vr[NDIM+1], fd, fdVal, rrinv;
  rrinv = 0.0;
  fd = 0.0;
  fdVal = 0.0;

  int start = 1 + rank*(cells[2]/size);
  int end = (rank+1)*(cells[2]/size);

  for(m1Y = start ; m1Y <= end ; m1Y ++){
    for(m1X = 1 ; m1X <= cells[1] ; m1X ++){
      m1 = (m1Y-1) * cells[1] + m1X + nAtom;
      for(offset = 1 ; offset <= 9 ; offset ++){
    m2X = m1X + iofX[offset]; shift[1] = 0.;
    if(m2X > cells[1]){
      m2X = 1; shift[1] = region[1];
    }else if(m2X == 0){
      m2X = cells[1]; shift[1] = -region[1];
    }
    m2Y = m1Y + iofY[offset]; shift[2] = 0.;
    if(m2Y > cells[2]){
      m2Y = 1; shift[2] = region[2];
    }else if(m2Y == 0){
      m2Y = cells[2]; shift[2] = -region[2];
    }
    m2 = (m2Y-1)*cells[1] + m2X + nAtom;
    I = cellList[m1];
    while(I > 0){
      J = cellList[m2];
      while(J > 0){
        if(m1 == m2 && J != I && (atomRadius[I] > 0. && atomRadius[J] > 0.)){
          dr[1] = rx[I] - rx[J] - shift[1];
          dr[2] = ry[I] - ry[J] - shift[2];
          rr = Sqr(dr[1]) + Sqr(dr[2]);
          RadiusIJ = atomRadius[I] + atomRadius[J];
          SqrRadiusIJ = Sqr(RadiusIJ);
          if(rr < SqrRadiusIJ){
        r = sqrt(rr);
        ri = 1.0/r;
                rrinv = 1.0/rr;
                vr[1] = vx[I] - vx[J];
                vr[2] = vy[I] - vy[J];
        RadiusIJInv = 1.0/RadiusIJ;
        uVal = Sqr(1.0 - r * RadiusIJInv);
        fcVal = 2.0 * RadiusIJInv * (1.0 - r * RadiusIJInv) *ri;
                fdVal = -gamman * (vr[1]*dr[1] + vr[2]*dr[2]) * rrinv; //disc-disc drag

        f  = fcVal * dr[1];
                fd = fdVal * dr[1];
        ax[I] += (f + fd);
                discDragx[I] += fd; //disc-disc drag

        f = fcVal * dr[2];
                fd = fdVal * dr[2];
        ay[I] += (f + fd);
                discDragy[I] += fd; //disc-disc drag

        uSum +=  0.5 * uVal;
        virSum += 0.5 * fcVal * rr;
        rfAtom += 0.5 * dr[1] * fcVal * dr[2];
          }
        }else if(m1 != m2 && (atomRadius[I] > 0. && atomRadius[J] > 0.)){
          dr[1] = rx[I] - rx[J] - shift[1];
          dr[2] = ry[I] - ry[J] - shift[2];
          rr = Sqr(dr[1]) + Sqr(dr[2]);
          RadiusIJ = atomRadius[I] + atomRadius[J];
          SqrRadiusIJ = Sqr(RadiusIJ);
          if(rr < SqrRadiusIJ){
        r = sqrt(rr);
        ri = 1.0/r;
                rrinv = 1.0/r;
                vr[1] = vx[I] - vx[J];
                vr[2] = vy[I] - vy[J];
        RadiusIJInv = 1.0/RadiusIJ;
        uVal = Sqr(1.0 - r * RadiusIJInv);
        fcVal = 2.0 * RadiusIJInv * (1.0 - r * RadiusIJInv) *ri;
                fdVal = -gamman * (vr[1]*dr[1] + vr[2]*dr[2]) * rrinv; //disc-disc drag

        f  = fcVal * dr[1];
                fd =  fdVal * dr[1];
        ax[I] += (f + fd);
                discDragx[I] += fd; //disc-disc drag

        f  = fcVal * dr[2];
                fd = fdVal * dr[2];
        ay[I] += (f + fd);
                discDragy[I] += fd; //disc-disc drag

        uSum +=  0.5 * uVal;
        virSum += 0.5 * fcVal * rr;
        rfAtom += 0.5 * dr[1] * fcVal * dr[2];
          }
        }
            J = cellList[J];
      }
      I = cellList[I];
    }
      }
    }
  }
}
```

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;
```

```
  Pairatom2[nPairActive] = atomIDj;
  PairXij[nPairActive] = dr[1];
  PairYij[nPairActive] = dr[2];

  //DampFlag = 1
  if(DampFlag == 1){
  meff = (atomMass[atomIDi]*atomMass[atomIDj])/(atomMass[atomIDi] + atomMass[atomIDj]);
  fdVal = -gamman * meff * (vr[1]*dr[1] + vr[2]*dr[2]) * rri; //disc-disc drag

  discDragx[atomIDi] =  fdVal * dr[1]; //disc-disc drag
  discDragy[atomIDi] =  fdVal * dr[2]; //disc-disc drag
  discDragx[atomIDj] = -fdVal * dr[1]; //disc-disc drag
  discDragy[atomIDj] = -fdVal * dr[2]; //disc-disc drag

  discDragx[nPairActive] = discDragx[atomIDi];
  discDragy[nPairActive] = discDragy[atomIDi];


  ax[atomIDi] += (fcVal + fdVal) * dr[1];
  ay[atomIDi] += (fcVal + fdVal) * dr[2];
  ax[atomIDj] += -(fcVal + fdVal) * dr[1];
  ay[atomIDj] += -(fcVal + fdVal) * dr[2];
 }

 //DampFlag = 2
 else if(DampFlag == 2){
  discDragx[atomIDi] =  -gamman * vr[1]; //disc-disc drag
  discDragy[atomIDi] =  -gamman * vr[2]; //disc-disc drag
  discDragx[atomIDj] = -(-gamman * vr[1]); //disc-disc drag
  discDragy[atomIDj] = -(-gamman * vr[2]); //disc-disc drag

  discDragx[nPairActive] = discDragx[atomIDi];
  discDragy[nPairActive] = discDragy[atomIDi];


  ax[atomIDi] +=  (fcVal * dr[1] - gamman * vr[1]);
  ay[atomIDi] +=  (fcVal * dr[2] - gamman * vr[2]);
  ax[atomIDj] += -(fcVal * dr[1] - gamman * vr[1]);
  ay[atomIDj] += -(fcVal * dr[2] - gamman * vr[2]);
 }

 //DampFlag = 3. Suzanne PRL, 130, 178203 (2023) version
 else if(DampFlag == 3){
 //Track compression velocity
 DeltaXijNew = dr[1];
 DeltaYijNew = dr[2];
 if(stepCount == 0) { // Initialization step
  DeltaXijOldPair[atomIDi][atomIDj] = DeltaXijNew;
  DeltaYijOldPair[atomIDi][atomIDj] = DeltaYijNew;
  }

  DeltaXij = DeltaXijNew - DeltaXijOldPair[atomIDi][atomIDj];
  DeltaYij = DeltaYijNew - DeltaYijOldPair[atomIDi][atomIDj];
  DeltaVXij = DeltaXij / deltaT;
  DeltaVYij = DeltaYij / deltaT;

  // Update history for next step
  DeltaXijOldPair[atomIDi][atomIDj] = DeltaXijNew;
  DeltaYijOldPair[atomIDi][atomIDj] = DeltaYijNew;

  discDragx[atomIDi] =  -gamman * DeltaVXij; //disc-disc drag
  discDragy[atomIDi] =  -gamman * DeltaVYij; //disc-disc drag
  discDragx[atomIDj] = -(-gamman * DeltaVXij); //disc-disc drag
  discDragy[atomIDj] = -(-gamman * DeltaVYij); //disc-disc drag

  discDragx[nPairActive] = discDragx[atomIDi];
  discDragy[nPairActive] = discDragy[atomIDi];

  ax[atomIDi] +=  (fcVal * dr[1] - gamman * DeltaVXij);
  ay[atomIDi] +=  (fcVal * dr[2] - gamman * DeltaVYij);
  ax[atomIDj] += -(fcVal * dr[1] - gamman * DeltaVXij);
  ay[atomIDj] += -(fcVal * dr[2] - gamman * DeltaVYij);
 }

 //In the following, for stress/virial term (fcVal + fdVal) is used since the total pair force =
Hookean Interaction + relative velocity drag
 uSumPair +=  0.5 * uVal;
 virSumPair += 0.5 * (fcVal + fdVal) * rr;
 virSumPairxx += 0.5 * (fcVal + fdVal) * dr[1] * dr[1];
 virSumPairyy += 0.5 * (fcVal + fdVal) * dr[2] * dr[2];
 virSumPairxy += 0.5 * (fcVal + fdVal) * dr[1] * dr[2];
   }
 else { //Resetting the distance between two discs when they are not in contact
  DeltaXijOldPair[atomIDi][atomIDj] = 0.0;
  DeltaYijOldPair[atomIDi][atomIDj] = 0.0;
  DeltaXijOldPair[atomIDj][atomIDi] = 0.0;
  DeltaYijOldPair[atomIDj][atomIDi] = 0.0;
```

```
    }
   }
  }
 }
}
```

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:

main
ComputePairForce

3.31 ComputePairForce.c

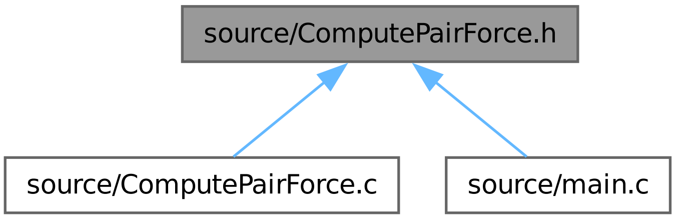
Go to the documentation of this file.

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

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

 */

#include "ComputePairForce.h"

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

void ComputePairForce(int normFlag){
double dr[NDIM+1], fcVal, rr, ri, r, uVal;
int n, i,j;
uVal = 0.0;  uSumPair = 0.0 ;
virSumPair = 0.0; virSumPairxx = 0.0; virSumPairyy = 0.0; virSumPairxy = 0.0;

for(n = 1 ; n <= nAtom ; n ++){
 ax[n] = 0.0;
 ay[n] = 0.0;
 discDragx[n] = 0.0;
 discDragy[n] = 0.0;
}
for(n = 1; n <= nPairTotal; n ++){
 PairID[n] = 0;
 Pairatom1[n] = 0;
 Pairatom2[n] = 0;
 PairXij[n] = 0.0;
 PairYij[n] = 0.0;
}


Kn = 1.0;
double vr[NDIM+1], fdVal, rri;
```

```
nPairActive = 0;
double meff;
meff = 0.0;
int atomIDi, atomIDj;
//int processThisPair = 1;

for(i=1;i<=nAtomInterface;i++){
 for(j=i+1;j<=nAtomInterface;j++){
  atomIDi = atomIDInterface[i];
  atomIDj = atomIDInterface[j];
  if (isBonded[atomIDi][atomIDj] == 0) { //To exclude pair interaction between bonded atoms
  rr = 0.0; rri = 0.0; fcVal = 0.0;  fdVal = 0.0; strech = 0.0;
  RadiusIJ = 0.0;

  dr[1] = rx[atomIDi] - rx[atomIDj];
  if(dr[1] >= regionH[1])
   dr[1] -= region[1];
  else if(dr[1] < -regionH[1])
    dr[1] += region[1];

  dr[2] = ry[atomIDi] - ry[atomIDj];
   if(dr[2] >= regionH[2]){
    dr[1] -= shearDisplacement;
    if(dr[1] < -regionH[1]) dr[1] += region[1];
    dr[2] -= region[2];
  }else if(dr[2] < -regionH[2]){
   dr[1] += shearDisplacement;
    if(dr[1] >= regionH[1]) dr[1] -= region[1];
   dr[2] += region[2];
  }

  rr = Sqr(dr[1]) + Sqr(dr[2]);
  RadiusIJ = atomRadius[atomIDi] + atomRadius[atomIDj];
  SqrRadiusIJ = Sqr(RadiusIJ);
  if(rr < SqrRadiusIJ){
   r = sqrt(rr);
   ri = 1.0/r;
   rri = 1.0/rr;
   RadiusIJInv = 1.0/RadiusIJ;
   strech = (RadiusIJ - r);
   uVal = 0.5 * Kn * Sqr(strech);

   //NormFlag
   if(normFlag == 1){
    strech = strech * RadiusIJInv;
    uVal = 0.5 * Kn * RadiusIJ * Sqr(strech);
    }

   fcVal = Kn * strech * ri;
   vr[1] = vx[atomIDi] - vx[atomIDj];
   vr[2] = vy[atomIDi] - vy[atomIDj];

   nPairActive++;
   PairID[nPairActive] = nPairActive;
   Pairatom1[nPairActive] = atomIDi;
   Pairatom2[nPairActive] = atomIDj;
   PairXij[nPairActive] = dr[1];
   PairYij[nPairActive] = dr[2];

   //DampFlag = 1
   if(DampFlag == 1){
   meff = (atomMass[atomIDi]*atomMass[atomIDj])/(atomMass[atomIDi] + atomMass[atomIDj]);
   fdVal = -gamman * meff * (vr[1]*dr[1] + vr[2]*dr[2]) * rri; //disc-disc drag

   discDragx[atomIDi] =  fdVal * dr[1]; //disc-disc drag
   discDragy[atomIDi] =  fdVal * dr[2]; //disc-disc drag
   discDragx[atomIDj] = -fdVal * dr[1]; //disc-disc drag
   discDragy[atomIDj] = -fdVal * dr[2]; //disc-disc drag

   discDragx[nPairActive] = discDragx[atomIDi];
   discDragy[nPairActive] = discDragy[atomIDi];


   ax[atomIDi] += (fcVal + fdVal) * dr[1];
   ay[atomIDi] += (fcVal + fdVal) * dr[2];
   ax[atomIDj] += -(fcVal + fdVal) * dr[1];
   ay[atomIDj] += -(fcVal + fdVal) * dr[2];
  }

  //DampFlag = 2
  else if(DampFlag == 2){
   discDragx[atomIDi] =  -gamman * vr[1]; //disc-disc drag
   discDragy[atomIDi] =  -gamman * vr[2]; //disc-disc drag
   discDragx[atomIDj] = -(-gamman * vr[1]); //disc-disc drag
   discDragy[atomIDj] = -(-gamman * vr[2]); //disc-disc drag

   discDragx[nPairActive] = discDragx[atomIDi];
   discDragy[nPairActive] = discDragy[atomIDi];


   ax[atomIDi] +=  (fcVal * dr[1] - gamman * vr[1]);
   ay[atomIDi] +=  (fcVal * dr[2] - gamman * vr[2]);
   ax[atomIDj] += -(fcVal * dr[1] - gamman * vr[1]);
   ay[atomIDj] += -(fcVal * dr[2] - gamman * vr[2]);
  }

  //DampFlag = 3. Suzanne PRL, 130, 178203 (2023) version
  else if(DampFlag == 3){
  //Track compression velocity
  DeltaXijNew = dr[1];
  DeltaYijNew = dr[2];
  if(stepCount == 0) { // Initialization step
   DeltaXijOldPair[atomIDi][atomIDj] = DeltaXijNew;
   DeltaYijOldPair[atomIDi][atomIDj] = DeltaYijNew;
   }

   DeltaXij = DeltaXijNew - DeltaXijOldPair[atomIDi][atomIDj];
   DeltaYij = DeltaYijNew - DeltaYijOldPair[atomIDi][atomIDj];
   DeltaVXij = DeltaXij / deltaT;
   DeltaVYij = DeltaYij / deltaT;

   // Update history for next step
   DeltaXijOldPair[atomIDi][atomIDj] = DeltaXijNew;
   DeltaYijOldPair[atomIDi][atomIDj] = DeltaYijNew;

   discDragx[atomIDi] =  -gamman * DeltaVXij; //disc-disc drag
   discDragy[atomIDi] =  -gamman * DeltaVYij; //disc-disc drag
   discDragx[atomIDj] = -(-gamman * DeltaVXij); //disc-disc drag
   discDragy[atomIDj] = -(-gamman * DeltaVYij); //disc-disc drag

   discDragx[nPairActive] = discDragx[atomIDi];
   discDragy[nPairActive] = discDragy[atomIDi];

   ax[atomIDi] +=  (fcVal * dr[1] - gamman * DeltaVXij);
   ay[atomIDi] +=  (fcVal * dr[2] - gamman * DeltaVYij);
   ax[atomIDj] += -(fcVal * dr[1] - gamman * DeltaVXij);
   ay[atomIDj] += -(fcVal * dr[2] - gamman * DeltaVYij);
  }

  //In the following, for stress/virial term (fcVal + fdVal) is used since the total pair force = Hookean Interaction + relative velocity drag
  uSumPair +=  0.5 * uVal;
  virSumPair += 0.5 * (fcVal + fdVal) * rr;
  virSumPairxx += 0.5 * (fcVal + fdVal) * dr[1] * dr[1];
  virSumPairyy += 0.5 * (fcVal + fdVal) * dr[2] * dr[2];
  virSumPairxy += 0.5 * (fcVal + fdVal) * dr[1] * dr[2];
    }
  else { //Resetting the distance between two discs when they are not in contact
   DeltaXijOldPair[atomIDi][atomIDj] = 0.0;
   DeltaYijOldPair[atomIDi][atomIDj] = 0.0;
   DeltaXijOldPair[atomIDj][atomIDi] = 0.0;
   DeltaYijOldPair[atomIDj][atomIDi] = 0.0;
    }
   }
  }
 }
}
```

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
```

```
dr[2] = ry[atomIDi] - ry[atomIDj];
 if(dr[2] >= regionH[2]){
  dr[1] -= shearDisplacement;
  if(dr[1] < -regionH[1]) dr[1] += region[1];
  dr[2] -= region[2];
}else if(dr[2] < -regionH[2]){
 dr[1] += shearDisplacement;
  if(dr[1] >= regionH[1]) dr[1] -= region[1];
 dr[2] += region[2];
}

rr = Sqr(dr[1]) + Sqr(dr[2]);
RadiusIJ = atomRadius[atomIDi] + atomRadius[atomIDj];
SqrRadiusIJ = Sqr(RadiusIJ);
if(rr < SqrRadiusIJ){
 r = sqrt(rr);
 ri = 1.0/r;
 rri = 1.0/rr;
 RadiusIJInv = 1.0/RadiusIJ;
 strech = (RadiusIJ - r);
 uVal = 0.5 * Kn * Sqr(strech);

 //NormFlag
 if(normFlag == 1){
  strech = strech * RadiusIJInv;
  uVal = 0.5 * Kn * RadiusIJ * Sqr(strech);
  }

 fcVal = Kn * strech * ri;
 vr[1] = vx[atomIDi] - vx[atomIDj];
 vr[2] = vy[atomIDi] - vy[atomIDj];

 nPairActive++;
 PairID[nPairActive] = nPairActive;
 Pairatom1[nPairActive] = atomIDi;
 Pairatom2[nPairActive] = atomIDj;
 PairXij[nPairActive] = dr[1];
 PairYij[nPairActive] = dr[2];

 //DampFlag = 1
 if(DampFlag == 1){
 meff = (atomMass[atomIDi]*atomMass[atomIDj])/(atomMass[atomIDi] + atomMass[atomIDj]);
 fdVal = -gamman * meff * (vr[1]*dr[1] + vr[2]*dr[2]) * rri; //disc-disc drag

 discDragx[atomIDi] =  fdVal * dr[1]; //disc-disc drag
 discDragy[atomIDi] =  fdVal * dr[2]; //disc-disc drag
 discDragx[atomIDj] = -fdVal * dr[1]; //disc-disc drag
 discDragy[atomIDj] = -fdVal * dr[2]; //disc-disc drag

 discDragx[nPairActive] = discDragx[atomIDi];
 discDragy[nPairActive] = discDragy[atomIDi];


 ax[atomIDi] += (fcVal + fdVal) * dr[1];
 ay[atomIDi] += (fcVal + fdVal) * dr[2];
 ax[atomIDj] += -(fcVal + fdVal) * dr[1];
 ay[atomIDj] += -(fcVal + fdVal) * dr[2];
}

//DampFlag = 2
else if(DampFlag == 2){
 discDragx[atomIDi] =  -gamman * vr[1]; //disc-disc drag
 discDragy[atomIDi] =  -gamman * vr[2]; //disc-disc drag
 discDragx[atomIDj] = -(-gamman * vr[1]); //disc-disc drag
 discDragy[atomIDj] = -(-gamman * vr[2]); //disc-disc drag

 discDragx[nPairActive] = discDragx[atomIDi];
 discDragy[nPairActive] = discDragy[atomIDi];


 ax[atomIDi] +=  (fcVal * dr[1] - gamman * vr[1]);
 ay[atomIDi] +=  (fcVal * dr[2] - gamman * vr[2]);
 ax[atomIDj] += -(fcVal * dr[1] - gamman * vr[1]);
 ay[atomIDj] += -(fcVal * dr[2] - gamman * vr[2]);
}

//DampFlag = 3. Suzanne PRL, 130, 178203 (2023) version
else if(DampFlag == 3){
//Track compression velocity
DeltaXijNew = dr[1];
DeltaYijNew = dr[2];
if(stepCount == 0) { // Initialization step
 DeltaXijOldPair[atomIDi][atomIDj] = DeltaXijNew;
 DeltaYijOldPair[atomIDi][atomIDj] = DeltaYijNew;
 }

 DeltaXij = DeltaXijNew - DeltaXijOldPair[atomIDi][atomIDj];
```

```
   DeltaYij = DeltaYijNew - DeltaYijOldPair[atomIDi][atomIDj];
   DeltaVXij = DeltaXij / deltaT;
   DeltaVYij = DeltaYij / deltaT;

   // Update history for next step
   DeltaXijOldPair[atomIDi][atomIDj] = DeltaXijNew;
   DeltaYijOldPair[atomIDi][atomIDj] = DeltaYijNew;

   discDragx[atomIDi] =  -gamman * DeltaVXij; //disc-disc drag
   discDragy[atomIDi] =  -gamman * DeltaVYij; //disc-disc drag
   discDragx[atomIDj] = -(-gamman * DeltaVXij); //disc-disc drag
   discDragy[atomIDj] = -(-gamman * DeltaVYij); //disc-disc drag

   discDragx[nPairActive] = discDragx[atomIDi];
   discDragy[nPairActive] = discDragy[atomIDi];

   ax[atomIDi] +=  (fcVal * dr[1] - gamman * DeltaVXij);
   ay[atomIDi] +=  (fcVal * dr[2] - gamman * DeltaVYij);
   ax[atomIDj] += -(fcVal * dr[1] - gamman * DeltaVXij);
   ay[atomIDj] += -(fcVal * dr[2] - gamman * DeltaVYij);
  }

  //In the following, for stress/virial term (fcVal + fdVal) is used since the total pair force = Hookean Interaction + relative velocity drag
  uSumPair +=  0.5 * uVal;
  virSumPair += 0.5 * (fcVal + fdVal) * rr;
  virSumPairxx += 0.5 * (fcVal + fdVal) * dr[1] * dr[1];
  virSumPairyy += 0.5 * (fcVal + fdVal) * dr[2] * dr[2];
  virSumPairxy += 0.5 * (fcVal + fdVal) * dr[1] * dr[2];
    }
  else { //Resetting the distance between two discs when they are not in contact
   DeltaXijOldPair[atomIDi][atomIDj] = 0.0;
   DeltaYijOldPair[atomIDi][atomIDj] = 0.0;
   DeltaXijOldPair[atomIDj][atomIDi] = 0.0;
   DeltaYijOldPair[atomIDj][atomIDi] = 0.0;
    }
   }
  }
 }
}
```

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:

main
ComputePairForce

3.33 ComputePairForce.h

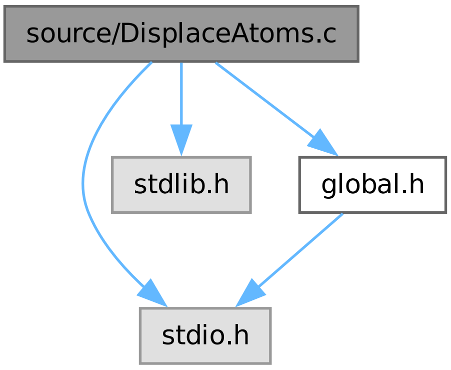
Go to the documentation of this file.

```
#ifndef COMPUTE_PAIR_FORCE_H
#define COMPUTE_PAIR_FORCE_H

void ComputePairForce(int normFlag);

#endif

```

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

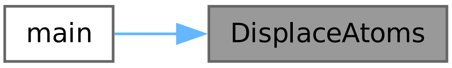
3.34.1.1 DisplaceAtoms()

```
void DisplaceAtoms ( )
```

Definition at line 25 of file DisplaceAtoms.c.

```
                      {
 int n;
  for(n = 1; n <= nAtom; n ++){
   if(molID[n] == 2){
    rx[n] += DeltaX;
    ry[n] += DeltaY;
} } }
```

References DeltaX, DeltaY, molID, nAtom, rx, and ry.
Referenced by main().
Here is the caller graph for this function:



3.35 DisplaceAtoms.c

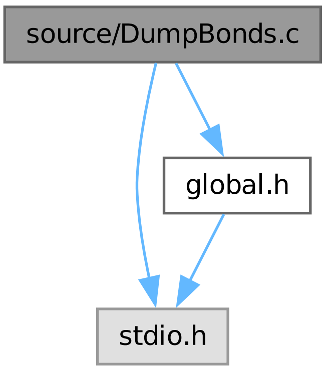
Go to the documentation of this file.

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

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

 */

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

void DisplaceAtoms(){
 int n;
  for(n = 1; n <= nAtom; n ++){
   if(molID[n] == 2){
    rx[n] += DeltaX;
    ry[n] += DeltaY;
} } }
```

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 ( )`

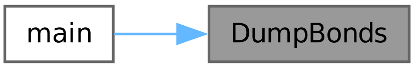
Definition at line 24 of file DumpBonds.c.

```
00024                  {
  int n;
  //Trajectory file in LAMMPS dump format for OVITO visualization
  fprintf(fpbond, "ITEM: TIMESTEP\n");
  fprintf(fpbond, "%lf\n",timeNow);
  fprintf(fpbond, "ITEM: NUMBER OF ENTRIES\n");
  fprintf(fpbond, "%d\n",nBond);
  fprintf(fpbond, "ITEM: BOX BOUNDS pp ff pp\n");
  fprintf(fpbond, "%lf %lf xlo xhi\n", -regionH[1], regionH[1]);
  fprintf(fpbond, "%lf %lf ylo yhi\n", -regionH[2], regionH[2]);
  fprintf(fpbond, "%lf %lf zlo zhi\n", -0.1, 0.1);
  fprintf(fpbond, "ITEM: ENTRIES BondID, BondType, atom1 atom2 BondLength BondLengthEqul nodeDragx1
nodeDragy1\n");

  for(n=1; n<=nBond; n++)
   fprintf(fpbond, "%d %d %d %d %0.16lf %0.16lf %0.16lf %0.16lf\n", BondID[n], BondType[n], atom1[n],
atom2[n],
   BondLength[n], ro[n], nodeDragx[atom1[n]], nodeDragy[atom1[n]]);
  }
```

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

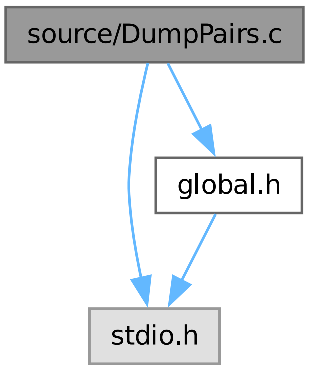
Go to the documentation of this file.

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

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

 */

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

void DumpBonds(){
  int n;
  //Trajectory file in LAMMPS dump format for OVITO visualization
  fprintf(fpbond, "ITEM: TIMESTEP\n");
  fprintf(fpbond, "%lf\n",timeNow);
  fprintf(fpbond, "ITEM: NUMBER OF ENTRIES\n");
  fprintf(fpbond, "%d\n",nBond);
  fprintf(fpbond, "ITEM: BOX BOUNDS pp ff pp\n");
  fprintf(fpbond, "%lf %lf xlo xhi\n", -regionH[1], regionH[1]);
  fprintf(fpbond, "%lf %lf ylo yhi\n", -regionH[2], regionH[2]);
  fprintf(fpbond, "%lf %lf zlo zhi\n", -0.1, 0.1);
  fprintf(fpbond, "ITEM: ENTRIES BondID, BondType, atom1 atom2 BondLength BondLengthEqul nodeDragx1
nodeDragy1\n");

  for(n=1; n<=nBond; n++)
   fprintf(fpbond, "%d %d %d %d %0.16lf %0.16lf %0.16lf %0.16lf\n", BondID[n], BondType[n], atom1[n],
atom2[n],
   BondLength[n], ro[n], nodeDragx[atom1[n]], nodeDragy[atom1[n]]);
  }



```

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 ( )
```

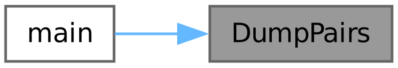
Definition at line 25 of file DumpPairs.c.

```
                   {
 int n;
 //Trajectory file in LAMMPS dump format for OVITO visualization
 fprintf(fppair, "ITEM: TIMESTEP\n");
 fprintf(fppair, "%lf\n",timeNow);
 fprintf(fppair, "ITEM: NUMBER OF ENTRIES\n");
 fprintf(fppair, "%d\n",nPairActive);
 fprintf(fppair, "ITEM: BOX BOUNDS pp ff pp\n");
 fprintf(fppair, "%lf %lf xlo xhi\n", -regionH[1], regionH[1]);
 fprintf(fppair, "%lf %lf ylo yhi\n", -regionH[2], regionH[2]);
 fprintf(fppair, "%lf %lf zlo zhi\n", -0.1, 0.1);
 fprintf(fppair, "ITEM: ENTRIES index, atom1 atom2 xij yij discDragx1 discDragy1\n");

 for(n=1; n<=nPairActive; n++)
  fprintf(fppair, "%d %d %d %0.16lf %0.16lf %0.16lf %0.16lf\n", PairID[n], Pairatom1[n],
Pairatom2[n],
  PairXij[n], PairYij[n], discDragx[n], discDragy[n]);

 }
```

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

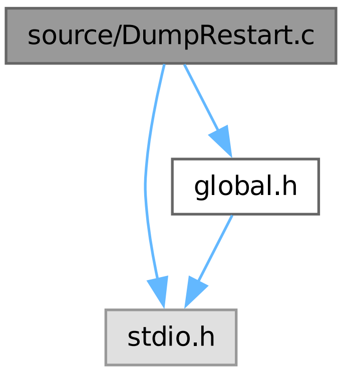
Go to the documentation of this file.

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

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

 */


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

void DumpPairs(){
  int n;
  //Trajectory file in LAMMPS dump format for OVITO visualization
  fprintf(fppair, "ITEM: TIMESTEP\n");
  fprintf(fppair, "%lf\n",timeNow);
  fprintf(fppair, "ITEM: NUMBER OF ENTRIES\n");
  fprintf(fppair, "%d\n",nPairActive);
  fprintf(fppair, "ITEM: BOX BOUNDS pp ff pp\n");
  fprintf(fppair, "%lf %lf xlo xhi\n", -regionH[1], regionH[1]);
  fprintf(fppair, "%lf %lf ylo yhi\n", -regionH[2], regionH[2]);
  fprintf(fppair, "%lf %lf zlo zhi\n", -0.1, 0.1);
  fprintf(fppair, "ITEM: ENTRIES index, atom1 atom2 xij yij discDragx1 discDragy1\n");

  for(n=1; n<=nPairActive; n++)
   fprintf(fppair, "%d %d %d %0.16lf %0.16lf %0.16lf %0.16lf\n", PairID[n], Pairatom1[n],
      Pairatom2[n],
   PairXij[n], PairYij[n], discDragx[n], discDragy[n]);

  }



```

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 ( )
```

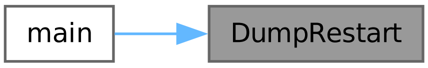
Definition at line 25 of file DumpRestart.c.

```
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:



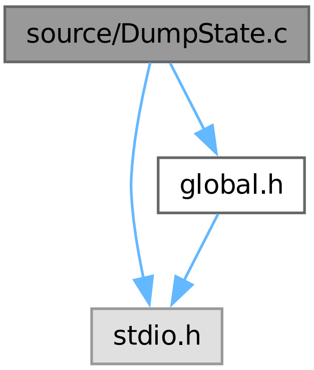
3.41 DumpRestart.c

Go to the documentation of this file.

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

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

 */


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

void DumpRestart() {
 char DUMP[256];
 FILE *fpDUMP;
 sprintf(DUMP, "%s.Restart", prefix);
 fpDUMP = fopen(DUMP, "w");
 if(fpDUMP == NULL) {
  fprintf(stderr, "Error opening file %s for writing\n", DUMP);
  return;
 }

  fprintf(fpDUMP, "timeNow %lf\n", timeNow);
  fprintf(fpDUMP, "nAtom %d\n",  nAtom);
  fprintf(fpDUMP, "nBond %d\n", nBond);
  fprintf(fpDUMP, "nAtomType %d\n", nAtomType);
  fprintf(fpDUMP, "nBondType %d\n", nBondType);
  fprintf(fpDUMP, "region[1] %0.14lf\n", region[1]);
  fprintf(fpDUMP, "region[2] %0.14lf\n", region[2]);

  int n;
  fprintf(fpDUMP, "Atoms\n");
  for(n = 1; n <= nAtom; n ++)
   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]);


  fprintf(fpDUMP, "Bonds\n");
  for(n=1; n<=nBond; n++)
  fprintf(fpDUMP,  "%d %d %d %d %0.2lf %0.16lf\n", BondID[n], BondType[n], atom1[n], atom2[n], kb[n],
ro[n]);

  fclose(fpDUMP);
}

```

3.42 source/DumpState.c File Reference

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



Functions

- void DumpState ()

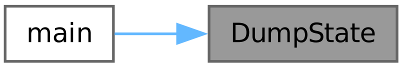
3.42.1 Function Documentation

3.42.1.1 DumpState()

```
void DumpState ( )
```
Definition at line 25 of file DumpState.c.

```
                  {
 char DUMP[256];
 FILE *fpDUMP;
 sprintf(DUMP, "%s.STATE", prefix);
 fpDUMP = fopen(DUMP, "w");
 if(fpDUMP == NULL) {
  fprintf(stderr, "Error opening file %s for writing\n", DUMP);
  return;
 }

  fprintf(fpDUMP, "ITEM: TIMESTEP\n");
  fprintf(fpDUMP, "%lf\n",timeNow);
  fprintf(fpDUMP, "ITEM: NUMBER OF ATOMS\n");
  fprintf(fpDUMP, "%d\n",nAtom);
  fprintf(fpDUMP, "ITEM: BOX BOUNDS pp pp pp\n");
  fprintf(fpDUMP, "%lf %lf xlo xhi\n", -regionH[1], regionH[1]);
  fprintf(fpDUMP, "%lf %lf ylo yhi\n", -regionH[2], regionH[2]);
  fprintf(fpDUMP, "%lf %lf zlo zhi\n",  -0.1, 0.1);
  fprintf(fpDUMP, "ITEM: ATOMS id mol type radius x y vx vy fx fy\n");
  int n;
  for (n = 1; n <= nAtom; n++) {
   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",
   atomID[n], molID[n], atomType[n], atomRadius[n], rx[n], ry[n], vx[n], vy[n], ax[n], ay[n]);
  }
  fclose(fpDUMP);
}
```
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.

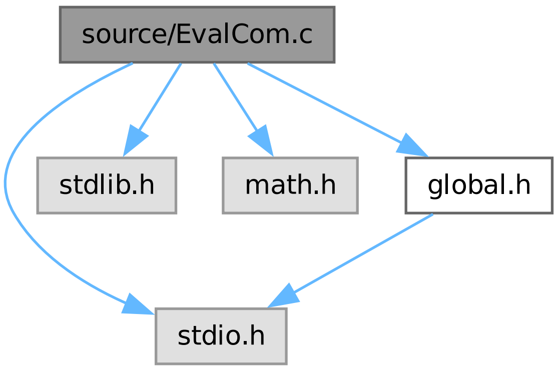
```
/*
 * This file is part of Lamina.
 *
 * Lamina is free software: you can redistribute it and/or modify
 * it under the terms of the GNU General Public License as published by
 * the Free Software Foundation, either version 3 of the License, or
 * (at your option) any later version.
 *
 * Lamina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

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

 */


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

void DumpState() {
 char DUMP[256];
 FILE *fpDUMP;
 sprintf(DUMP, "%s.STATE", prefix);
 fpDUMP = fopen(DUMP, "w");
 if(fpDUMP == NULL) {
  fprintf(stderr, "Error opening file %s for writing\n", DUMP);
  return;
 }

  fprintf(fpDUMP, "ITEM: TIMESTEP\n");
  fprintf(fpDUMP, "%lf\n",timeNow);
  fprintf(fpDUMP, "ITEM: NUMBER OF ATOMS\n");
  fprintf(fpDUMP, "%d\n",nAtom);
  fprintf(fpDUMP, "ITEM: BOX BOUNDS pp pp pp\n");
  fprintf(fpDUMP, "%lf %lf xlo xhi\n", -regionH[1], regionH[1]);
  fprintf(fpDUMP, "%lf %lf ylo yhi\n", -regionH[2], regionH[2]);
  fprintf(fpDUMP, "%lf %lf zlo zhi\n",  -0.1, 0.1);
  fprintf(fpDUMP, "ITEM: ATOMS id mol type radius x y vx vy fx fy\n");
  int n;
  for (n = 1; n <= nAtom; n++) {
   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",
   atomID[n], molID[n], atomType[n], atomRadius[n], rx[n], ry[n], vx[n], vy[n], ax[n], ay[n]);
  }
  fclose(fpDUMP);
}

```

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 ( )
```

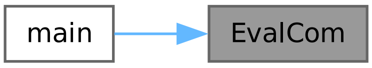
Definition at line 27 of file EvalCom.c.

```
               {
 int n;
 ComX = 0.0; ComY = 0.0; ComXRatio = 0.0; ComYRatio = 0.0;
 TotalMass = 0.0;

 for(n=1; n<=nAtom; n++){
 if(molID[n] == 2){
  ComX += atomMass[n] * rxUnwrap[n];
  ComY += atomMass[n] * ryUnwrap[n];
  TotalMass += atomMass[n];
  } }

  ComX = ComX/TotalMass;
  ComY = ComY/TotalMass;

  if(timeNow == 0.0){
  ComX0 = ComX; ComY0 = ComY;
  }
  ComXRatio = ComX/ComX0;   ComYRatio = ComY/ComY0;
 }
```

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

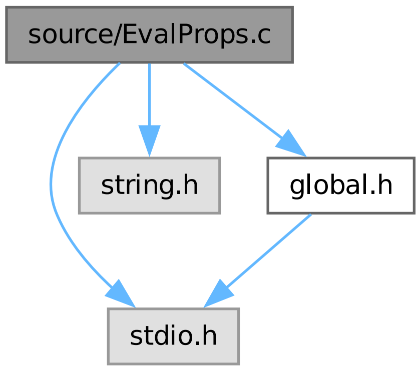
Go to the documentation of this file.

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

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

 */


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

void EvalCom(){
 int n;
 ComX = 0.0; ComY = 0.0; ComXRatio = 0.0; ComYRatio = 0.0;
 TotalMass = 0.0;

 for(n=1; n<=nAtom; n++){
 if(molID[n] == 2){
  ComX += atomMass[n] * rxUnwrap[n];
  ComY += atomMass[n] * ryUnwrap[n];
  TotalMass += atomMass[n];
  } }

  ComX = ComX/TotalMass;
  ComY = ComY/TotalMass;

  if(timeNow == 0.0){
  ComX0 = ComX; ComY0 = ComY;
  }
  ComXRatio = ComX/ComX0;   ComYRatio = ComY/ComY0;
 }



```

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.

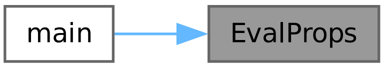
```
00026                       {
00027  real v, vv;
00028  virSum = 0.0;
00029  vSumX = 0.0; vSumY = 0.0; vSum = 0.0;
00030  vvSum = 0.;
00031  int n;
00032
00033  for (n = 1; n <= nAtom; n++) {
00034   vv = 0.;
00035   // Initialize v with a default value to avoid "uninitialized" warning.
00036   v = 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 ;
```

```
  virSum = virSumPair + virSumBond;
  pressure = density * (vvSum + virSum) / (nAtom * NDIM);

}
```

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.

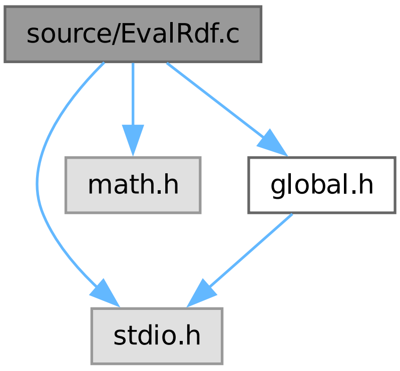
```
/*
 * This file is part of Lamina.
 *
 * Lamina is free software: you can redistribute it and/or modify
 * it under the terms of the GNU General Public License as published by
 * the Free Software Foundation, either version 3 of the License, or
 * (at your option) any later version.
 *
 * Lamina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

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

 */


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

void EvalProps() {
 real v, vv;
 virSum = 0.0;
 vSumX = 0.0; vSumY = 0.0; vSum = 0.0;
 vvSum = 0.;
 int n;

 for (n = 1; n <= nAtom; n++) {
  vv = 0.;
  // Initialize v with a default value to avoid "uninitialized" warning.
  v = 0.0;
  // X direction velocity
  if (strcmp(solver, "Verlet") == 0) {
    v = vx[n];
  } else if (strcmp(solver, "LeapFrog") == 0) {
    v = vx[n] - 0.5 * deltaT * ax[n];
  }
   vSum += v;
   vv += Sqr(v);
   vSumX += v;
   // Y direction velocity
   if (strcmp(solver, "Verlet") == 0) {
   v = vy[n];
   } else if (strcmp(solver, "LeapFrog") == 0) {
   v = vy[n] - 0.5 * deltaT * ay[n];
   }
```

```
    vSum += v;
    vSumY += v;
    vv += Sqr(v);
    vvSum += vv;
  }

  kinEnergy = 0.5 * vvSum / nAtom ;
  uSumPairPerAtom = uSumPair / nAtom ;
  BondEnergyPerAtom = TotalBondEnergy / (0.5*nAtom); //Factor of 0.5 since each atom has one half the
      bond energy
  potEnergy = uSumPairPerAtom +  BondEnergyPerAtom ;
  totEnergy = kinEnergy + potEnergy;
  virSumxx = virSumPairxx  + virSumBondxx ;
  virSumyy = virSumPairyy  + virSumBondyy ;
  virSumxy = virSumPairxy  + virSumBondxy ;
  virSum = virSumPair + virSumBond;
  pressure = density * (vvSum + virSum) / (nAtom * NDIM);

}

```

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.

```
                    {
  real dr[NDIM+1], deltaR, normFac, rr, rrRange;
  int j1, j2, n;
  countRdf ++;
  if(countRdf == 1){
    for(n = 1 ; n <= sizeHistRdf ; n ++)
      histRdf[n] = 0.;
  }
  rrRange = Sqr(rangeRdf);
  deltaR = rangeRdf / sizeHistRdf;
  for(j1 = 1 ; j1 <= nAtom - 1 ; j1 ++){
    for(j2 = j1 + 1 ; j2 <= nAtom ; j2 ++){

      dr[1] = rx[j1] - rx[j2];
      if(fabs(dr[1]) > regionH[1])
    dr[1] -= SignR(region[1], dr[1]);

      dr[2] = ry[j1] - ry[j2];
      if(fabs(dr[2]) > regionH[2])
    dr[2] -= SignR(region[2], dr[2]);

      rr = Sqr(dr[1]) + Sqr(dr[2]);

      if(rr < rrRange){
    n = (int)(sqrt(rr)/deltaR) + 1;
    histRdf[n] ++;
      }
    }
  }

  if(countRdf == limitRdf){
    normFac = region[1]*region[2] / (M_PI*Sqr(deltaR)*nAtom*nAtom*countRdf );
    for(n = 1 ; n <= sizeHistRdf ; n ++)
      histRdf[n] *= normFac/(n-0.5);
    // PRINT THE RADIAL DISTRIBUTION DATA ON TO DISK FILE
    real rBin;
    int n;
    fprintf(fprdf,"rdf @ timeNow %lf\n", timeNow);
    for(n = 1 ; n <= sizeHistRdf ; n ++){
      rBin = (n - 0.5)*rangeRdf/sizeHistRdf;
      fprintf(fprdf, "%lf %lf\n", rBin, histRdf[n]);
    }
  }

}
```

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.

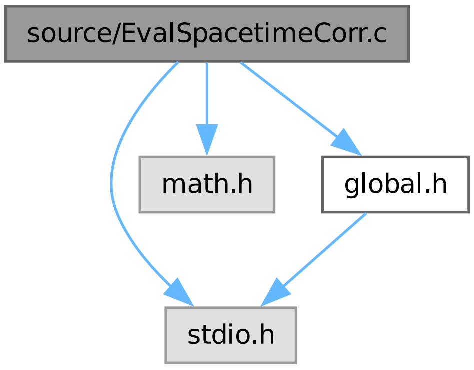
```
/*
 * This file is part of Lamina.
 *
 * Lamina is free software: you can redistribute it and/or modify
 * it under the terms of the GNU General Public License as published by
 * the Free Software Foundation, either version 3 of the License, or
 * (at your option) any later version.
 *
 * Lamina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

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

 */


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

void EvalRdf(){
  real dr[NDIM+1], deltaR, normFac, rr, rrRange;
  int j1, j2, n;
  countRdf ++;
  if(countRdf == 1){
    for(n = 1 ; n <= sizeHistRdf ; n ++)
      histRdf[n] = 0.;
  }
  rrRange = Sqr(rangeRdf);
  deltaR = rangeRdf / sizeHistRdf;
  for(j1 = 1 ; j1 <= nAtom - 1 ; j1 ++){
    for(j2 = j1 + 1 ; j2 <= nAtom ; j2 ++){

      dr[1] = rx[j1] - rx[j2];
      if(fabs(dr[1]) > regionH[1])
    dr[1] -= SignR(region[1], dr[1]);

```

```
      dr[2] = ry[j1] - ry[j2];
      if(fabs(dr[2]) > regionH[2])
    dr[2] -= SignR(region[2], dr[2]);

      rr = Sqr(dr[1]) + Sqr(dr[2]);

      if(rr < rrRange){
    n = (int)(sqrt(rr)/deltaR) + 1;
    histRdf[n] ++;
      }
    }
  }

  if(countRdf == limitRdf){
    normFac = region[1]*region[2] / (M_PI*Sqr(deltaR)*nAtom*nAtom*countRdf );
    for(n = 1 ; n <= sizeHistRdf ; n ++)
      histRdf[n] *= normFac/(n-0.5);
    // PRINT THE RADIAL DISTRIBUTION DATA ON TO DISK FILE
    real rBin;
    int n;
    fprintf(fprdf,"rdf @ timeNow %lf\n", timeNow);
    for(n = 1 ; n <= sizeHistRdf ; n ++){
      rBin = (n - 0.5)*rangeRdf/sizeHistRdf;
      fprintf(fprdf, "%lf %lf\n", rBin, histRdf[n]);
    }
  }

}

```

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                            {
```

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

for (j = 1; j <= 2*nFunCorr; j++)
  cfVal[j] = 0.;

for (n = 1; n <= nAtom; n++){
  j = 1;
  COSA = cos(kMin*rx[n]);
  SINA = sin(kMin*rx[n]);
  for (m = 1; m <= nFunCorr; m++){
    if(m == 1){
  cosV = cos(deltaK*rx[n]);
  sinV = sin(deltaK*rx[n]);
  cosV0 = cosV;
    }else if(m == 2){
  cosV1 = cosV;
  sinV1 = sinV;
  cosV = 2.*cosV0*cosV1-1;
  sinV = 2.*cosV0*sinV1;
    }else{
  cosV2 = cosV1;
  sinV2 = sinV1;
  cosV1 = cosV;
  sinV1 = sinV;
  cosV = 2.*cosV0*cosV1-cosV2;
  sinV = 2.*cosV0*sinV1-sinV2;
    }
    COSV = COSA*cosV - SINA*sinV;
    SINV = SINA*cosV + COSA*sinV;
    cfVal[j] += COSV;
    cfVal[j+1] += SINV;
    j += 2;
  }
}

for (nb = 1; nb <= nBuffCorr; nb++){
  indexCorr[nb] += 1;
  if (indexCorr[nb] <= 0) continue;
  ni = nFunCorr * (indexCorr[nb] - 1);
  if (indexCorr[nb] == 1){
    for (j = 1; j <= 2*nFunCorr; j++)
  cfOrg[nb][j] = cfVal[j];
  }

  for (j = 1; j <= nFunCorr; j++)
    spacetimeCorr[nb][ni + j] = 0.;

  j = 1;
  for (m = 1; m <= nFunCorr; m++){
    nv = m + ni;
    spacetimeCorr[nb][nv] += cfVal[j] * cfOrg[nb][j] + cfVal[j + 1] * cfOrg[nb][j + 1];
    j += 2;
  }

}

// ACCUMULATE SPACETIME CORRELATIONS
for (nb = 1; nb <= nBuffCorr; nb++){
 if (indexCorr[nb] == nValCorr){
   for (j = 1; j <= nFunCorr*nValCorr; j++)
     spacetimeCorrAv[j] += spacetimeCorr[nb][j];
   indexCorr[nb] = 0.;
   countCorrAv ++;
   if (countCorrAv == limitCorrAv){
     for (j = 1; j <= nFunCorr*nValCorr; j++)
   spacetimeCorrAv[j] /= (nAtom*limitCorrAv);
     fprintf(fpdnsty,"NDIM %d\n", NDIM);
     fprintf(fpdnsty,"nAtom %d\n", nAtom);
     fprintf(fpdnsty,"region %lf\n", region[1]);
     fprintf(fpdnsty,"nFunCorr %d\n", nFunCorr);
     fprintf(fpdnsty,"limitCorrAv %d\n", limitCorrAv);
     fprintf(fpdnsty,"stepCorr %d\n", stepCorr);
     fprintf(fpdnsty,"nValCorr %d\n", nValCorr);
     fprintf(fpdnsty,"deltaT %lf\n", deltaT);
     real tVal;
     for (n = 1; n <= nValCorr; n++){
   tVal = (n-1)*stepCorr*deltaT;
   fprintf (fpdnsty, "%e\t", tVal);
   int nn = nFunCorr*(n-1);
   for (j = 1; j <= nFunCorr; j ++)
         fprintf (fpdnsty, "%e\t", spacetimeCorrAv[nn + j]);
       fprintf (fpdnsty, "\n");
```

```
      }

      countCorrAv = 0.;
      for (j = 1; j <= nFunCorr*nValCorr; j++)
    spacetimeCorrAv[j] = 0.;
    }
  }
 }
}
```

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

3.51 EvalSpacetimeCorr.c

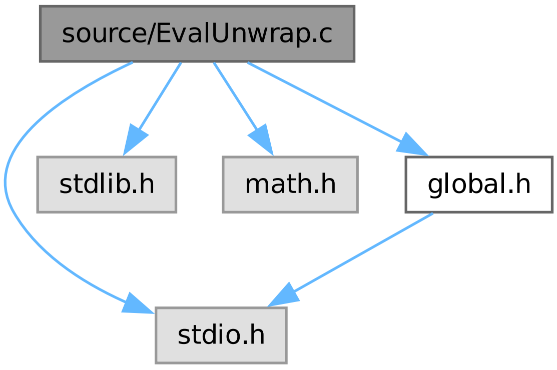
Go to the documentation of this file.

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

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

 */


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

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

  for (j = 1; j <= 2*nFunCorr; j++)
    cfVal[j] = 0.;

  for (n = 1; n <= nAtom; n++){
    j = 1;
    COSA = cos(kMin*rx[n]);
    SINA = sin(kMin*rx[n]);
    for (m = 1; m <= nFunCorr; m++){
      if(m == 1){
    cosV = cos(deltaK*rx[n]);
    sinV = sin(deltaK*rx[n]);
    cosV0 = cosV;
      }else if(m == 2){
    cosV1 = cosV;
    sinV1 = sinV;
    cosV = 2.*cosV0*cosV1-1;
    sinV = 2.*cosV0*sinV1;
      }else{
    cosV2 = cosV1;
    sinV2 = sinV1;
    cosV1 = cosV;
    sinV1 = sinV;
    cosV = 2.*cosV0*cosV1-cosV2;
    sinV = 2.*cosV0*sinV1-sinV2;
      }
      COSV = COSA*cosV - SINA*sinV;
      SINV = SINA*cosV + COSA*sinV;
      cfVal[j] += COSV;
      cfVal[j+1] += SINV;
      j += 2;
    }
  }

  for (nb = 1; nb <= nBuffCorr; nb++){
    indexCorr[nb] += 1;
    if (indexCorr[nb] <= 0) continue;
    ni = nFunCorr * (indexCorr[nb] - 1);
    if (indexCorr[nb] == 1){
      for (j = 1; j <= 2*nFunCorr; j++)
    cfOrg[nb][j] = cfVal[j];
    }

    for (j = 1; j <= nFunCorr; j++)
      spacetimeCorr[nb][ni + j] = 0.;

    j = 1;
    for (m = 1; m <= nFunCorr; m++){
      nv = m + ni;
      spacetimeCorr[nb][nv] += cfVal[j] * cfOrg[nb][j] + cfVal[j + 1] * cfOrg[nb][j + 1];
      j += 2;
    }

  }

  // ACCUMULATE SPACETIME CORRELATIONS
  for (nb = 1; nb <= nBuffCorr; nb++){
   if (indexCorr[nb] == nValCorr){
     for (j = 1; j <= nFunCorr*nValCorr; j++)
       spacetimeCorrAv[j] += spacetimeCorr[nb][j];
     indexCorr[nb] = 0.;
     countCorrAv ++;
     if (countCorrAv == limitCorrAv){
       for (j = 1; j <= nFunCorr*nValCorr; j++)
     spacetimeCorrAv[j] /= (nAtom*limitCorrAv);
       fprintf(fpdnsty,"NDIM %d\n", NDIM);
       fprintf(fpdnsty,"nAtom %d\n", nAtom);
       fprintf(fpdnsty,"region %lf\n", region[1]);
       fprintf(fpdnsty,"nFunCorr %d\n", nFunCorr);
       fprintf(fpdnsty,"limitCorrAv %d\n", limitCorrAv);
       fprintf(fpdnsty,"stepCorr %d\n", stepCorr);
       fprintf(fpdnsty,"nValCorr %d\n", nValCorr);
       fprintf(fpdnsty,"deltaT %lf\n", deltaT);
       real tVal;
       for (n = 1; n <= nValCorr; n++){
     tVal = (n-1)*stepCorr*deltaT;
     fprintf (fpdnsty, "%e\t", tVal);
     int nn = nFunCorr*(n-1);
     for (j = 1; j <= nFunCorr; j ++)
           fprintf (fpdnsty, "%e\t", spacetimeCorrAv[nn + j]);
         fprintf (fpdnsty, "\n");
       }

       countCorrAv = 0.;
       for (j = 1; j <= nFunCorr*nValCorr; j++)
     spacetimeCorrAv[j] = 0.;
     }
   }
  }
}
```

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

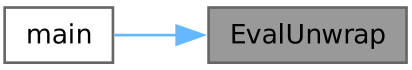
3.52.1.1 EvalUnwrap()

```
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.

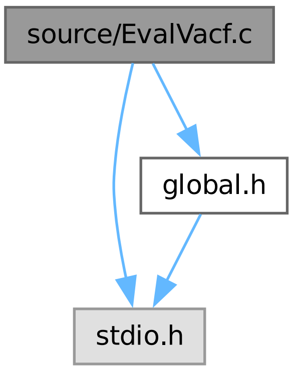
```
00001 /*
00002  * This file is part of Lamina.
00003  *
00004  * Lamina is free software: you can redistribute it and/or modify
00005  * it under the terms of the GNU General Public License as published by
00006  * the Free Software Foundation, either version 3 of the License, or
```

```
 * (at your option) any later version.
 *
 * Lamina is distributed in the hope that it will be useful,
 * but WITHOUT ANY WARRANTY; without even the implied warranty of
 * MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the
 * GNU General Public License for more details.
 *
 * You should have received a copy of the GNU General Public License
 * along with Lamina. If not, see <https://www.gnu.org/licenses/>.

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

 */


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

void EvalUnwrap() {
 int n;
 for (n = 1; n <= nAtom; n++) {
  rxUnwrap[n] = rx[n] + ImageX[n] * region[1];
  ryUnwrap[n] = ry[n] + ImageY[n] * region[2];
  }
}
```

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.

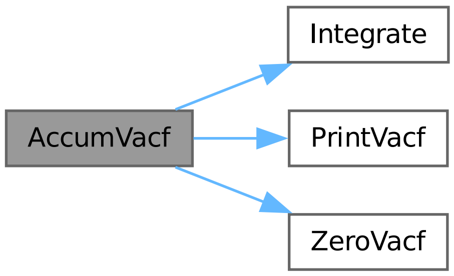
```
00027                 {
00028  double fac;
```

```
 int j, nb;
 for(nb = 1 ; nb <= nBuffAcf ; nb ++){
  if(indexAcf[nb] == nValAcf){
   for(j = 1 ; j <= nValAcf; j ++){
    viscAcfAv[j] +=  viscAcf[nb][j];
    }
  indexAcf[nb] = 0;
  countAcfAv ++;
  if(countAcfAv == limitAcfAv){
   fac = 1./(kinEnergy*region[1]*region[2]*limitAcfAv);
   viscAcfInt = fac*stepAcf*deltaT*Integrate(viscAcfAv, nValAcf);
   PrintVacf();
   ZeroVacf();
} } } }
```

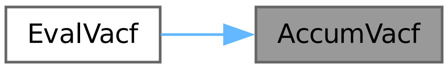
References countAcfAv, deltaT, indexAcf, Integrate(), kinEnergy, limitAcfAv, nBuffAcf, nValAcf, PrintVacf(), region, stepAcf, viscAcf, viscAcfAv, viscAcfInt, and ZeroVacf().

Referenced by EvalVacf().

Here is the call graph for this function:



Here is the caller graph for this function:



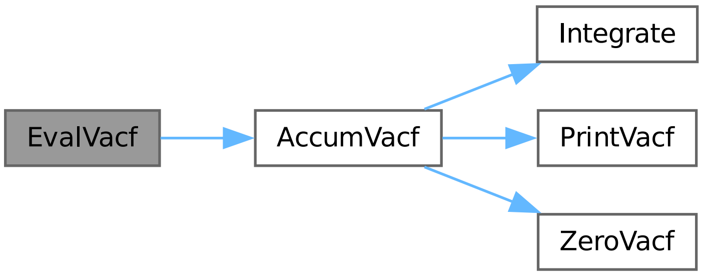
3.54.1.2 EvalVacf()

```
void EvalVacf ( )
```

Definition at line 26 of file EvalVacf.c.

```
                {
 int n, nb, ni;
 double viscVec = 0.;
 double v[3];
 for(n = 1 ; n <= nAtom ; n ++){
   v[1] = vx[n] - 0.5*ax[n]*deltaT;
   v[2] = vy[n] - 0.5*ay[n]*deltaT;
   viscVec += v[1]*v[2];
 }
 viscVec += rfAtom;
 for(nb = 1 ; nb <= nBuffAcf ; nb ++){
   indexAcf[nb] ++;
   if(indexAcf[nb] <= 0)continue;
   if(indexAcf[nb] == 1){
      viscAcfOrg[nb] = viscVec;
    }
    ni = indexAcf[nb];
    viscAcf[nb][ni] = viscAcfOrg[nb]*viscVec;
  }
  AccumVacf();
}
```

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

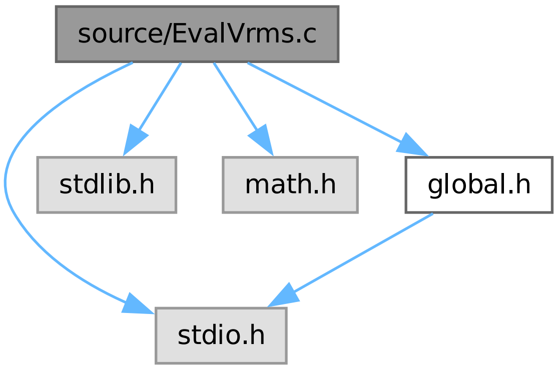
Go to the documentation of this file.

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

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

 */


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

void AccumVacf();
void EvalVacf(){
  int n, nb, ni;
  double viscVec = 0.;
  double v[3];
  for(n = 1 ; n <= nAtom ; n ++){
    v[1] = vx[n] - 0.5*ax[n]*deltaT;
    v[2] = vy[n] - 0.5*ay[n]*deltaT;
    viscVec += v[1]*v[2];
  }
  viscVec += rfAtom;
  for(nb = 1 ; nb <= nBuffAcf ; nb ++){
    indexAcf[nb] ++;
    if(indexAcf[nb] <= 0)continue;
    if(indexAcf[nb] == 1){
      viscAcfOrg[nb] = viscVec;
    }
    ni = indexAcf[nb];
    viscAcf[nb][ni] = viscAcfOrg[nb]*viscVec;
  }
  AccumVacf();
}
```

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 ( )
```

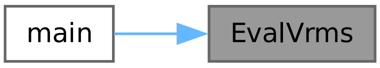
Definition at line 27 of file EvalVrms.c.

```
               {
  int n;
  VSqr = 0.0;
  VMeanSqr = 0.0;
  VRootMeanSqr = 0.0;

  for(n = 1 ; n <= nAtom ; n ++){
  VSqr += Sqr(vx[n]) + Sqr(vy[n]);
  }
  VMeanSqr = VSqr/nAtom;
  VRootMeanSqr = sqrt(VMeanSqr);
  }
```

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

Referenced by main().

Here is the caller graph for this function:



3.57 EvalVrms.c

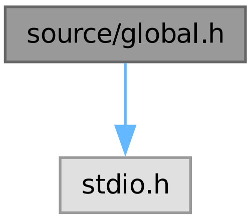
Go to the documentation of this file.

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

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

 */


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

void EvalVrms(){
  int n;
  VSqr = 0.0;
  VMeanSqr = 0.0;
  VRootMeanSqr = 0.0;

  for(n = 1 ; n <= nAtom ; n ++){
  VSqr += Sqr(vx[n]) + Sqr(vy[n]);
  }
  VMeanSqr = VSqr/nAtom;
  VRootMeanSqr = sqrt(VMeanSqr);
  }



```

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 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]
- 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.

```
#ifndef GLOBAL_H
#define GLOBAL_H
#include <stdio.h>  // Required for FILE*

#ifdef DEFINE_GLOBALS
    #define EXTERN
#else
    #define EXTERN extern
#endif
```

```c

typedef double real;

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

EXTERN double *rx, *ry, *vx, *vy, *ax, *ay;
EXTERN double *speed;

EXTERN double region[NDIM+1], regionH[NDIM+1], deltaT, timeNow, potEnergy, kinEnergy, totEnergy,
density, pressure, rCut, kappa, uSum, virSum, svirSum, vSum, vSumX, vSumY, vvSum, sPotEnergy,
 sKinEnergy,
sTotEnergy, sPressure, ssPotEnergy, ssKinEnergy, ssTotEnergy, ssPressure;

EXTERN int     initUcell[NDIM+1], moreCycles, nAtom, stepAvg, stepCount, stepEquil, stepLimit,
 stepTraj, stepDump;

EXTERN double  RadiusIJ, SqrRadiusIJ, RadiusIJInv;
EXTERN int     nAtomType;
EXTERN int     *atomType;
EXTERN int     *atomID;
EXTERN double  *atomRadius;
EXTERN double  *atomMass, TotalMass;

EXTERN int     nBond, nBondType;
EXTERN int     *atom1, *atom2;
EXTERN int     *BondID, *BondType ;
EXTERN double  *kb, *ro;
EXTERN double  *BondEnergy, *BondLength;
EXTERN double  TotalBondEnergy, BondEnergyPerAtom;
EXTERN double  gamman;
EXTERN double  *discDragx, *discDragy, *nodeDragx, *nodeDragy;
EXTERN double  strain, strainRate;
EXTERN double  shearDisplacement, shearVelocity;
EXTERN double  VSqr, VMeanSqr, VRootMeanSqr;
EXTERN double  ComX, ComY, ComX0, ComY0, ComXRatio, ComYRatio;
EXTERN double  HaltCondition;
EXTERN double  DeltaY, DeltaX;
EXTERN int     *ImageX, *ImageY;
EXTERN double  *rxUnwrap, *ryUnwrap;
EXTERN int     nAtomInterface, nDiscInterface,  nAtomBlock;
EXTERN int     *atomIDInterface;
EXTERN double  Kn;
EXTERN double  fx, fy, FyBylx, fxByfy;
EXTERN int     DampFlag;
EXTERN double  strech;

//For dumping the pair interaction data
EXTERN int     dumpPairFlag;
EXTERN int     nPairTotal, nPairActive;
EXTERN int     *PairID, *Pairatom1, *Pairatom2;
EXTERN double  *PairXij, *PairYij;


EXTERN char   solver[128];
EXTERN char   xBoundary[10], yBoundary[10];
EXTERN char     thermo;

//For damping as in PRL, 130, 178203 (2023)
EXTERN double *DeltaXijOld, *DeltaYijOld;
EXTERN double DeltaXijNew, DeltaYijNew;
EXTERN double DeltaXij, DeltaYij, DeltaVXij, DeltaVYij;
EXTERN double **DeltaXijOldPair, **DeltaYijOldPair;

//For molecule-ID as per LAMMPS, helpful!
EXTERN int    *molID;
EXTERN int    **isBonded;

//Following three for MPI only
EXTERN int     *cellList, cells[NDIM+1];
EXTERN int     rank, size, master;
EXTERN double  *fax, *fay, fuSum, fvirSum, frfAtom;

//For thermodynamic properties
EXTERN double  uSumPair, uSumPairPerAtom, virSumPair, virSumPairxx, virSumPairyy, virSumPairxy;
EXTERN double  virSumBond, virSumBondxx, virSumBondyy, virSumBondxy;
EXTERN double  virSumxx, virSumyy, virSumxy;
EXTERN int     freezeAtomType;

// Spacetime Correlations
EXTERN double  **cfOrg, **spacetimeCorr, *cfVal, *spacetimeCorrAv;
EXTERN int     *indexCorr, countCorrAv, limitCorrAv, nBuffCorr, nFunCorr, nValCorr, stepCorr;

// Viscosity
EXTERN double  rfAtom, frfAtom;
EXTERN double  *indexAcf, **viscAcf, *viscAcfOrg, *viscAcfAv, viscAcfInt;
EXTERN int      nValAcf, nBuffAcf, stepAcf, countAcfAv, limitAcfAv;

// Radial distribution function
EXTERN double  *histRdf, rangeRdf;
EXTERN int     countRdf, limitRdf, sizeHistRdf, stepRdf;


// Output files prefixes
EXTERN char      *prefix;

EXTERN char     result[250];
EXTERN FILE     *fpresult;

EXTERN char     xyz[256];
EXTERN FILE     *fpxyz;

EXTERN char     bond[256];
EXTERN FILE     *fpbond;


EXTERN char     dump[256];
EXTERN FILE     *fpdump;

EXTERN char     dnsty[256];
EXTERN FILE     *fpdnsty;

EXTERN char     visc[256];
EXTERN FILE     *fpvisc;

EXTERN char     rdf[256];
EXTERN FILE     *fprdf;

EXTERN char     vrms[256];
EXTERN FILE     *fpvrms;

EXTERN char     stress[256];
EXTERN FILE     *fpstress;

EXTERN char     momentum[256];
EXTERN FILE     *fpmomentum;

EXTERN char     com[256];
EXTERN FILE     *fpcom;

EXTERN char     pair[256];
EXTERN FILE     *fppair;

#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.

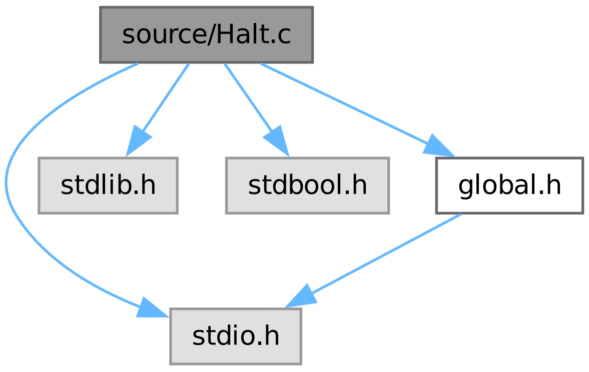
```
00001 #ifndef GLOBALEXTERN_H
00002 #define GLOBALEXTERN_H
00003
00004 typedef double real;
00005
00006 #define NDIM 2
00007 #define Sqr(x) ((x) * (x))
00008 #define SignR(x, y) (((y) >= 0) ? (x) : (- (x)))
00009
00010 extern double   *rx, *ry, *vx, *vy, *ax, *ay;
00011 extern double   *speed;
00012
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;
```

```

//Following three for MPI only
extern int     *cellList, cells[NDIM+1];
extern int     rank, size, master;
extern double  *fax, *fay, fuSum, fvirSum, frfAtom;

//For thermodynamic properties
extern double  uSumPair, uSumPairPerAtom, virSumPair, virSumPairxx, virSumPairyy, virSumPairxy;
extern double  virSumBond, virSumBondxx, virSumBondyy, virSumBondxy;
extern double  virSumxx, virSumyy, virSumxy;
extern int     freezeAtomType;

// Spacetime Correlations
extern double  **cfOrg, **spacetimeCorr, *cfVal, *spacetimeCorrAv;
extern int     *indexCorr, countCorrAv, limitCorrAv, nBuffCorr, nFunCorr, nValCorr, stepCorr;

// Viscosity
extern double  rfAtom, frfAtom;
extern double  *indexAcf, **viscAcf, *viscAcfOrg, *viscAcfAv, viscAcfInt;
extern int      nValAcf, nBuffAcf, stepAcf, countAcfAv, limitAcfAv;

// Radial distribution function
extern double  *histRdf, rangeRdf;
extern int     countRdf, limitRdf, sizeHistRdf, stepRdf;


// Output files prefixes
extern char    *prefix;

extern char    result[250];
extern FILE    *fpresult;

extern char    xyz[256];
extern FILE    *fpxyz;

extern char    bond[256];
extern FILE    *fpbond;


extern char    dump[256];
extern FILE    *fpdump;

extern char    dnsty[256];
extern FILE    *fpdnsty;

extern char    visc[256];
extern FILE    *fpvisc;

extern char    rdf[256];
extern FILE    *fprdf;

extern char    vrms[256];
extern FILE    *fpvrms;

extern char    stress[256];
extern FILE    *fpstress;

extern char    momentum[256];
extern FILE    *fpmomentum;

extern char    com[256];
extern FILE    *fpcom;

extern char    pair[256];
extern FILE    *fppair;

#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.

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

References fpresult, HaltCondition, and stepCount.
Referenced by main().
Here is the caller graph for this function:

main
HaltConditionCheck

3.63 Halt.c

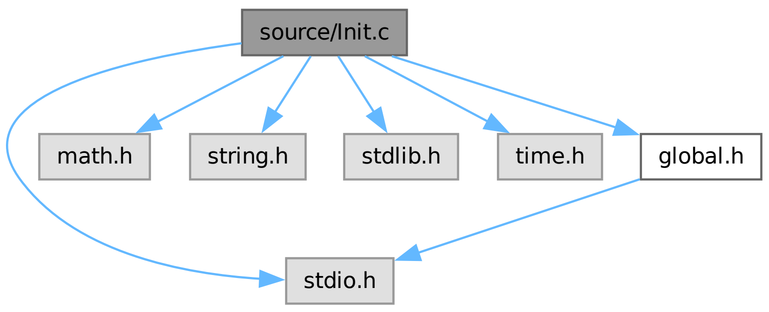
Go to the documentation of this file.

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

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

 */


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

bool HaltConditionCheck(double value, int stepCount) {

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

```

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));
```

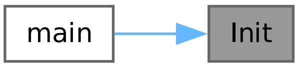
```
  atomMass = (double*)malloc((nAtom + 1) * sizeof(double));
  speed = (double*)malloc((nAtom + 1) * sizeof(double));
  atom1 = (int*)malloc((nBond+1)*sizeof(int));
  atom2 = (int*)malloc((nBond+1)*sizeof(int));
  BondID = (int*)malloc((nBond+1)*sizeof(int));
  BondType = (int*)malloc((nBond+1)*sizeof(int));
  kb = (double*)malloc((nBond+1)*sizeof(double));
  ro = (double*)malloc((nBond+1)*sizeof(double));
  BondEnergy = (double*)malloc((nBond+1)*sizeof(double));
  BondLength =(double*)malloc((nBond+1)*sizeof(double));
  discDragx = (double*)malloc((nAtom + 1) * sizeof(double));
  discDragy = (double*)malloc((nAtom + 1) * sizeof(double));
  nodeDragx = (double*)malloc((nAtom + 1) * sizeof(double));
  nodeDragy = (double*)malloc((nAtom + 1) * sizeof(double));
  ImageX = (int*)malloc((nAtom+1) * sizeof(int));
  ImageY = (int*)malloc((nAtom+1) * sizeof(int));
  rxUnwrap = (double*)malloc((nAtom + 1) * sizeof(double));
  ryUnwrap = (double*)malloc((nAtom + 1) * sizeof(double));
  DeltaXijOld = (double*)malloc((nBond+1)*sizeof(double));
  DeltaYijOld = (double*)malloc((nBond+1)*sizeof(double));
  DeltaXijOldPair = (double**)malloc((nAtom+1) * sizeof(double*));
  DeltaYijOldPair = (double**)malloc((nAtom+1) * sizeof(double*));
  for(int n = 0; n <= nAtom; n++) {
   DeltaXijOldPair[n] = (double*)malloc((nAtom+1) * sizeof(double));
   DeltaYijOldPair[n] = (double*)malloc((nAtom+1) * sizeof(double));
  }
  molID = (int*)malloc((nAtom+1) * sizeof(int));

  for(n = 1; n <= nAtom; n ++){
   atomMass[n] = 1.0;
  }

  fscanf(fpSTATE, "%s\n", dummy);
  for(n = 1; n <= nAtom; n ++)
   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]);


  fscanf(fpSTATE, "%s\n", dummy);
  for(n=1; n<=nBond; n++)
   fscanf(fpSTATE, "%d %d %d %d %lf %lf\n", &BondID[n], &BondType[n], &atom1[n], &atom2[n], &kb[n],
&ro[n]);

  fclose(fpSTATE);

 //2D-List of bonded atoms. This is used to remove pair interaction
 //calculation for the bonded atoms
   isBonded = (int**)malloc((nAtom + 1) * sizeof(int*));
  for (int i = 0; i <= nAtom; i++) {
    isBonded[i] = (int*)malloc((nAtom + 1) * sizeof(int));
    for (int j = 0; j <= nAtom; j++) {
        isBonded[i][j] = 0;
    }
  }

  for (n = 1; n <= nBond; n++) {
    int i = atom1[n];
    int j = atom2[n];
    isBonded[i][j] = 1;
    isBonded[j][i] = 1; // symmetric
}

 //For thermostate, update in final version
thermo = 'C';


 // List the interface atoms
 nAtomInterface = 0;
 nAtomBlock = 0;
 nDiscInterface = 0;
 double InterfaceWidth, bigDiameter;
 bigDiameter = 2.8;
 InterfaceWidth = 5.0 * bigDiameter;

 for(n = 1; n <= nAtom; n++){
  if(fabs(ry[n]) < InterfaceWidth){
  nAtomInterface++;
  }
  if(molID[n] == 2){
  nAtomBlock++;
  }
  if(atomRadius[n] != 0.0){
  nDiscInterface++;
  } }

   atomIDInterface =  (int*)malloc((nAtomInterface+1)*sizeof(int));

```

```c
  int m;
  m = 1;
  for(n=1; n<=nAtom; n++){
   if(fabs(ry[n]) < InterfaceWidth){
   atomIDInterface[m] = atomID[n];
   m++;
   } }

  nPairTotal = 0.5 * nAtomInterface * (nAtomInterface-1);
  PairID = (int*)malloc((nPairTotal+1) * sizeof(int));
  Pairatom1 = (int*)malloc((nPairTotal+1) * sizeof(int));
  Pairatom2 = (int*)malloc((nPairTotal+1) * sizeof(int));
  PairXij = (double*)malloc((nPairTotal+1) * sizeof(double));
  PairYij = (double*)malloc((nPairTotal+1) * sizeof(double));

    fprintf(fpresult, "------------------------------------\n");
    fprintf(fpresult, "-------PARAMETERS-----------\n");
    fprintf(fpresult, "------------------------------------\n");
    fprintf(fpresult, "nAtom\t\t\t%d\n",  nAtom);
    fprintf(fpresult, "nBond\t\t\t%d\n",  nBond);
    fprintf(fpresult, "nAtomBlock\t\t%d\n",  nAtomBlock);
    fprintf(fpresult, "nAtomInterface\t%d\n",  nAtomInterface);
    fprintf(fpresult, "nDiscInterface\t\t%d\n",  nDiscInterface);
    fprintf(fpresult, "gamman\t\t\t%0.6g\n", gamman);
    fprintf(fpresult, "strain\t\t\t%0.6g\n", strain);
    fprintf(fpresult, "strainRate\t\t%0.6g\n", strainRate);
    fprintf(fpresult, "FyBylx\t\t\t%0.6g\n", FyBylx);
    fprintf(fpresult, "fxByfy\t\t\t%0.6g\n", fxByfy);
    fprintf(fpresult, "DeltaY\t\t\t%0.6g\n", DeltaY);
    fprintf(fpresult, "DeltaX\t\t\t%0.6g\n", DeltaX);
    fprintf(fpresult, "HaltCondition\t\t%0.6g\n", HaltCondition);
    fprintf(fpresult, "kappa\t\t\t%g\n", kappa);
    fprintf(fpresult, "density\t\t\t%g\n", density);
    fprintf(fpresult, "rCut\t\t\t%g\n", rCut);
    fprintf(fpresult, "deltaT\t\t\t%g\n", deltaT);
    fprintf(fpresult, "stepEquil\t\t\t%d\n",  stepEquil);
    fprintf(fpresult, "stepLimit\t\t\t%d\n",  stepLimit);
    fprintf(fpresult, "region[1]\t\t\t%0.16lf\n", region[1]);
    fprintf(fpresult, "region[2]\t\t\t%0.16lf\n", region[2]);
    fprintf(fpresult, "cells[1]\t\t\t%d\n",  cells[1]);
    fprintf(fpresult, "cells[2]\t\t\t%d\n",  cells[2]);
    fprintf(fpresult, "solver\t\t\t%s\n",  solver);
    fprintf(fpresult, "boundary\t\t\t%s %s\n", xBoundary, yBoundary);
    fprintf(fpresult, "DampFlag\t\t\t%d\n",  DampFlag);


    fprintf(fpresult, "------------------------------------\n");
    fprintf(fpresult, "#TimeNow TotalMomentum PotEngyPerAtom KinEngyPerAtom TotEngyPerAtom PairEnergyPerAtom BondEnergyPerAtom  Press VirialSum\n");
    fprintf(fpvrms, "#timeNow\tVrms \n");
    fprintf(fpcom, "#timeNow\tComX\tComY\n");

/* //Uncomment the following as per your acquirement
    fprintf(fpstress, "strain           %lf\n", strain);
    fprintf(fpstress, "region[1]        %lf\n", region[1]);
    fprintf(fpstress, "region[2]        %lf\n", region[2]);
    fprintf(fpstress, "#timeNow virSumxx virSumyy virSumxy pressure\n");
    fprintf(fpmomentum, "#timeNow Px Py\n");
*/

   if((strcmp(xBoundary, "p") != 0 && strcmp(xBoundary, "r") != 0) ||
    (strcmp(yBoundary, "p") != 0 && strcmp(yBoundary, "r") != 0)) {
    fprintf(fpresult, "Error: Invalid boundary value detected: '%s %s'. Only 'p' or 'r' are allowed.\n", xBoundary, yBoundary);
    exit(EXIT_FAILURE); // Exit with failure status
  }

}
```

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.

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

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

 */


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

void Init(){
  char dummy[128];
  char inputConfig[128];
  FILE *fp;
  fp = fopen("input-data","r");
  fscanf(fp, "%s %s", dummy, inputConfig);
  fscanf(fp, "%s %s", dummy, solver);
  fscanf(fp, "%s %s %s", dummy, xBoundary, yBoundary);
  fscanf(fp, "%s %d",  dummy, &DampFlag);
  fscanf(fp, "%s %d",  dummy, &freezeAtomType);
  fscanf(fp, "%s %lf", dummy, &rCut);
  fscanf(fp, "%s %lf", dummy, &gamman);
  fscanf(fp, "%s %lf", dummy, &kappa);
  fscanf(fp, "%s %lf", dummy, &deltaT);
  fscanf(fp, "%s %lf", dummy, &strain);
  fscanf(fp, "%s %lf", dummy, &FyBylx);
  fscanf(fp, "%s %lf", dummy, &fxByfy);
  fscanf(fp, "%s %lf", dummy, &DeltaY);
  fscanf(fp, "%s %lf", dummy, &DeltaX);
  fscanf(fp, "%s %lf", dummy, &HaltCondition);
  fscanf(fp, "%s %d",  dummy, &stepAvg);
  fscanf(fp, "%s %d",  dummy, &stepEquil);
  fscanf(fp, "%s %d",  dummy, &stepLimit);
  fscanf(fp, "%s %d",  dummy, &stepDump);
  fscanf(fp, "%s %d",  dummy, &stepTraj);
  fscanf(fp, "%s %d",  dummy, &limitCorrAv);
  fscanf(fp, "%s %d",  dummy, &nBuffCorr);
  fscanf(fp, "%s %d",  dummy, &nFunCorr);
  fscanf(fp, "%s %d",  dummy, &nValCorr);
  fscanf(fp, "%s %d",  dummy, &stepCorr);
  fscanf(fp, "%s %d",  dummy, &limitAcfAv);
  fscanf(fp, "%s %d",  dummy, &nBuffAcf);
  fscanf(fp, "%s %d",  dummy, &nValAcf);
  fscanf(fp, "%s %d",  dummy, &stepAcf);
  fscanf(fp, "%s %lf", dummy, &rangeRdf);
```

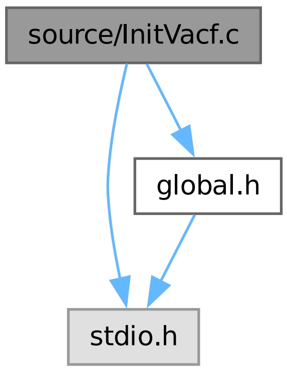
```c
fscanf(fp, "%s %d",  dummy, &limitRdf);
fscanf(fp, "%s %d",  dummy, &sizeHistRdf);
fscanf(fp, "%s %d",  dummy, &stepRdf);

fclose(fp);
FILE *fpSTATE;
if((fpSTATE = fopen(inputConfig,"r"))==NULL){
printf("Error occurred: Could not open STATE file\n Exiting now..\n");
exit(0);
}

fscanf(fpSTATE, "%s %lf", dummy, &timeNow);
fscanf(fpSTATE, "%s %d",  dummy, &nAtom);
fscanf(fpSTATE, "%s %d",  dummy, &nBond);
fscanf(fpSTATE, "%s %d",  dummy, &nAtomType);
fscanf(fpSTATE, "%s %d",  dummy, &nBondType);
fscanf(fpSTATE, "%s %lf", dummy, &region[1]);
fscanf(fpSTATE, "%s %lf", dummy, &region[2]);

region[2] *= 1.5; //Remove this when put on GitHub

density = nAtom/(region[1]*region[2]);
cells[1] = region[1] / rCut;
cells[2] = region[2] / rCut;
cellList = (int*)malloc((nAtom + cells[1] * cells[2] + 1) * sizeof(int));
regionH[1] = 0.5*region[1];
regionH[2] = 0.5*region[2];

//strain information
strainRate = strain/deltaT;
shearDisplacement = strain * region[2];
shearVelocity = strainRate * region[2];
int n;

rx = (double*)malloc((nAtom + 1) * sizeof(double));
ry = (double*)malloc((nAtom + 1) * sizeof(double));
vx = (double*)malloc((nAtom + 1) * sizeof(double));
vy = (double*)malloc((nAtom + 1) * sizeof(double));
ax = (double*)malloc((nAtom + 1) * sizeof(double));
ay = (double*)malloc((nAtom + 1) * sizeof(double));
fax = (double*)malloc((nAtom + 1) * sizeof(double));
fay = (double*)malloc((nAtom + 1) * sizeof(double));
atomID = (int*)malloc((nAtom+1) * sizeof(int));
atomType = (int*)malloc((nAtom+1) * sizeof(int));
atomRadius = (double*)malloc((nAtom + 1) * sizeof(double));
atomMass = (double*)malloc((nAtom + 1) * sizeof(double));
speed = (double*)malloc((nAtom + 1) * sizeof(double));
atom1 = (int*)malloc((nBond+1)*sizeof(int));
atom2 = (int*)malloc((nBond+1)*sizeof(int));
BondID = (int*)malloc((nBond+1)*sizeof(int));
BondType = (int*)malloc((nBond+1)*sizeof(int));
kb = (double*)malloc((nBond+1)*sizeof(double));
ro = (double*)malloc((nBond+1)*sizeof(double));
BondEnergy = (double*)malloc((nBond+1)*sizeof(double));
BondLength =(double*)malloc((nBond+1)*sizeof(double));
discDragx = (double*)malloc((nAtom + 1) * sizeof(double));
discDragy = (double*)malloc((nAtom + 1) * sizeof(double));
nodeDragx = (double*)malloc((nAtom + 1) * sizeof(double));
nodeDragy = (double*)malloc((nAtom + 1) * sizeof(double));
ImageX = (int*)malloc((nAtom+1) * sizeof(int));
ImageY = (int*)malloc((nAtom+1) * sizeof(int));
rxUnwrap = (double*)malloc((nAtom + 1) * sizeof(double));
ryUnwrap = (double*)malloc((nAtom + 1) * sizeof(double));
DeltaXijOld = (double*)malloc((nBond+1)*sizeof(double));
DeltaYijOld = (double*)malloc((nBond+1)*sizeof(double));
DeltaXijOldPair = (double**)malloc((nAtom+1) * sizeof(double*));
DeltaYijOldPair = (double**)malloc((nAtom+1) * sizeof(double*));
for(int n = 0; n <= nAtom; n++) {
 DeltaXijOldPair[n] = (double*)malloc((nAtom+1) * sizeof(double));
 DeltaYijOldPair[n] = (double*)malloc((nAtom+1) * sizeof(double));
}
molID = (int*)malloc((nAtom+1) * sizeof(int));

for(n = 1; n <= nAtom; n ++){
 atomMass[n] = 1.0;
}

fscanf(fpSTATE, "%s\n", dummy);
for(n = 1; n <= nAtom; n ++)
 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]);


fscanf(fpSTATE, "%s\n", dummy);
for(n=1; n<=nBond; n++)
 fscanf(fpSTATE, "%d %d %d %d %lf %lf\n", &BondID[n], &BondType[n], &atom1[n], &atom2[n], &kb[n],
&ro[n]);
```

```

  fclose(fpSTATE);

 //2D-List of bonded atoms. This is used to remove pair interaction
 //calculation for the bonded atoms
   isBonded = (int**)malloc((nAtom + 1) * sizeof(int*));
  for (int i = 0; i <= nAtom; i++) {
    isBonded[i] = (int*)malloc((nAtom + 1) * sizeof(int));
    for (int j = 0; j <= nAtom; j++) {
        isBonded[i][j] = 0;
    }
  }

  for (n = 1; n <= nBond; n++) {
    int i = atom1[n];
    int j = atom2[n];
    isBonded[i][j] = 1;
    isBonded[j][i] = 1; // symmetric
}

 //For thermostate, update in final version
thermo = 'C';


 // List the interface atoms
 nAtomInterface = 0;
 nAtomBlock = 0;
 nDiscInterface = 0;
 double InterfaceWidth, bigDiameter;
 bigDiameter = 2.8;
 InterfaceWidth = 5.0 * bigDiameter;

 for(n = 1; n <= nAtom; n++){
  if(fabs(ry[n]) < InterfaceWidth){
  nAtomInterface++;
  }
  if(molID[n] == 2){
  nAtomBlock++;
  }
  if(atomRadius[n] != 0.0){
  nDiscInterface++;
  } }

   atomIDInterface =  (int*)malloc((nAtomInterface+1)*sizeof(int));

  int m;
  m = 1;
  for(n=1; n<=nAtom; n++){
   if(fabs(ry[n]) < InterfaceWidth){
   atomIDInterface[m] = atomID[n];
   m++;
   } }

  nPairTotal = 0.5 * nAtomInterface * (nAtomInterface-1);
  PairID = (int*)malloc((nPairTotal+1) * sizeof(int));
  Pairatom1 = (int*)malloc((nPairTotal+1) * sizeof(int));
  Pairatom2 = (int*)malloc((nPairTotal+1) * sizeof(int));
  PairXij = (double*)malloc((nPairTotal+1) * sizeof(double));
  PairYij = (double*)malloc((nPairTotal+1) * sizeof(double));

    fprintf(fpresult, "------------------------------------\n");
    fprintf(fpresult, "-------PARAMETERS-----------\n");
    fprintf(fpresult, "------------------------------------\n");
    fprintf(fpresult, "nAtom\t\t\t%d\n",  nAtom);
    fprintf(fpresult, "nBond\t\t\t%d\n",  nBond);
    fprintf(fpresult, "nAtomBlock\t\t%d\n",  nAtomBlock);
    fprintf(fpresult, "nAtomInterface\t%d\n",  nAtomInterface);
    fprintf(fpresult, "nDiscInterface\t\t%d\n",  nDiscInterface);
    fprintf(fpresult, "gamman\t\t\t%0.6g\n", gamman);
    fprintf(fpresult, "strain\t\t\t%0.6g\n", strain);
    fprintf(fpresult, "strainRate\t\t%0.6g\n", strainRate);
    fprintf(fpresult, "FyBylx\t\t\t%0.6g\n", FyBylx);
    fprintf(fpresult, "fxByfy\t\t\t%0.6g\n", fxByfy);
    fprintf(fpresult, "DeltaY\t\t\t%0.6g\n", DeltaY);
    fprintf(fpresult, "DeltaX\t\t\t%0.6g\n", DeltaX);
    fprintf(fpresult, "HaltCondition\t\t%0.6g\n", HaltCondition);
    fprintf(fpresult, "kappa\t\t\t%g\n", kappa);
    fprintf(fpresult, "density\t\t\t%g\n", density);
    fprintf(fpresult, "rCut\t\t\t%g\n", rCut);
    fprintf(fpresult, "deltaT\t\t\t%g\n", deltaT);
    fprintf(fpresult, "stepEquil\t\t\t%d\n",  stepEquil);
    fprintf(fpresult, "stepLimit\t\t\t%d\n",  stepLimit);
    fprintf(fpresult, "region[1]\t\t\t%0.16lf\n", region[1]);
    fprintf(fpresult, "region[2]\t\t\t%0.16lf\n", region[2]);
    fprintf(fpresult, "cells[1]\t\t\t%d\n",  cells[1]);
    fprintf(fpresult, "cells[2]\t\t\t%d\n",  cells[2]);
    fprintf(fpresult, "solver\t\t\t%s\n",  solver);
    fprintf(fpresult, "boundary\t\t\t%s %s\n", xBoundary, yBoundary);
    fprintf(fpresult, "DampFlag\t\t%d\n",  DampFlag);


    fprintf(fpresult, "------------------------------------\n");
    fprintf(fpresult, "#TimeNow TotalMomentum PotEngyPerAtom KinEngyPerAtom TotEngyPerAtom
      PairEnergyPerAtom BondEnergyPerAtom  Press VirialSum\n");
    fprintf(fpvrms, "#timeNow\tVrms \n");
    fprintf(fpcom, "#timeNow\tComX\tComY\n");

/* //Uncomment the following as per your acquirement
    fprintf(fpstress, "strain           %lf\n", strain);
    fprintf(fpstress, "region[1]        %lf\n", region[1]);
    fprintf(fpstress, "region[2]        %lf\n", region[2]);
    fprintf(fpstress, "#timeNow virSumxx virSumyy virSumxy pressure\n");
    fprintf(fpmomentum, "#timeNow Px Py\n");
*/

   if((strcmp(xBoundary, "p") != 0 && strcmp(xBoundary, "r") != 0) ||
    (strcmp(yBoundary, "p") != 0 && strcmp(yBoundary, "r") != 0)) {
    fprintf(fpresult, "Error: Invalid boundary value detected: '%s %s'. Only 'p' or 'r' are
      allowed.\n", xBoundary, yBoundary);
    exit(EXIT_FAILURE); // Exit with failure status
  }

}
```

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()

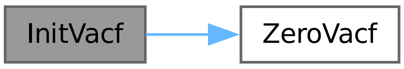
```
void InitVacf ( )
```

Definition at line 26 of file InitVacf.c.

```
                {
  int nb;
  for(nb = 1 ; nb <= nBuffAcf ; nb ++)
    indexAcf[nb] = -(nb-1)*nValAcf/nBuffAcf;
```

```
 ZeroVacf();
}
```

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:

main
SetupJob
InitVacf

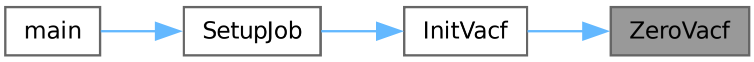
3.66.1.2 ZeroVacf()

```
void ZeroVacf ( )
```

Definition at line 25 of file ZeroVacf.c.

```
                {
int j;
countAcfAv= 0 ;
for(j = 1 ; j <= nValAcf ; j ++)
 viscAcfAv[j] = 0.;
}
```

Referenced by InitVacf().
Here is the caller graph for this function:



3.67 InitVacf.c

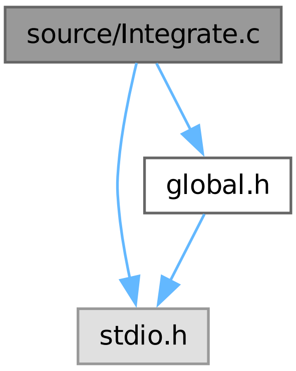
Go to the documentation of this file.

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

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

 */


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

void ZeroVacf();
void InitVacf(){
  int nb;
  for(nb = 1 ; nb <= nBuffAcf ; nb ++)
    indexAcf[nb] = -(nb-1)*nValAcf/nBuffAcf;
  ZeroVacf();
}
```

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 )
```

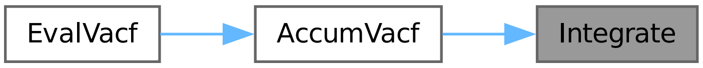
Definition at line 25 of file Integrate.c.

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

```
  s += f[i];
 return(s);
}
```

Referenced by AccumVacf().

Here is the caller graph for this function:



3.69 Integrate.c

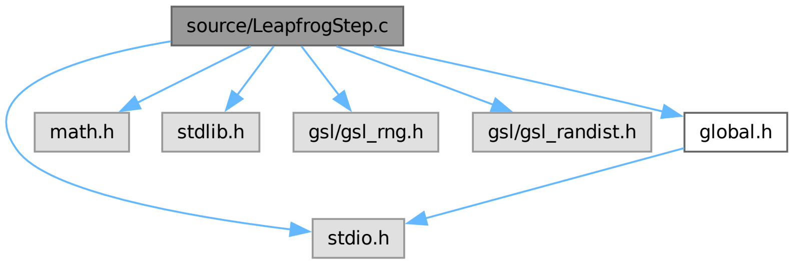
Go to the documentation of this file.

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

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

 */


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

double Integrate(double *f, int nf){
 double s;
 int i;
 s = 0.5*(f[1] + f[nf]);
 for(i = 2 ; i <= nf - 1 ; i ++)
  s += f[i];
 return(s);
}

```

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.

```
                                                 {
double temperature, GAMMA;
GAMMA = 100;

double *TValSum;
TValSum = (double*)malloc((nAtom + 1) * sizeof(double));


  if(stepCount <= stepEquil){
    double gSum, varS, massS;
    temperature = 1./GAMMA;

   if(stepCount == 1) varS = 0.;
    double A, S1, S2, T;
    int n;
    S1 = 0.; S2 = 0.; gSum = 0.; massS = 0.1;

    vvSum = 0.;
    double halfdt = 0.5*deltaT;
    for (n = 1; n <= nAtom; n++){
      T = vx[n] + halfdt * ax[n];
      S1 += T * ax[n];
      S2 += Sqr(T);

      T = vy[n] + halfdt * ay[n];
      S1 += T * ay[n];
      S2 += Sqr(T);
     vvSum += (Sqr(vx[n]) +  Sqr(vy[n]));
    }

    A = -S1 / S2;
    S2 = vvSum;

    double C = 1 + A*deltaT ;
    double D = deltaT * (1 + 0.5 * A * deltaT);

    int i,j;
    real dr[NDIM+1], r, rr, ri, rrCut;
    double vv;

    double uVal, AA, AASum;
    double TVal;

    double deno, VVSum;
    deno = 0.;
    VVSum = 0.;
    AASum = 0.;

  for(n=1;n<=nAtom; n++)
     TValSum[n] = 0.;

  rrCut = Sqr(rCut);

/*****Calculating Configarational temperature*****/
//Solving the equation of motion here
if(thermo == 'C'){
for(i = 1 ; i <= nAtom; i ++){
    for(j = i+1 ; j <= nAtom ; j ++){
      dr[1] = rx[i] - rx[j];
      if(fabs(dr[1]) > regionH[1])
    dr[1] -= SignR(region[1], dr[1]);

     dr[2] = ry[i] - ry[j];
      if(fabs(dr[2]) > regionH[2])
    dr[2] -= SignR(region[2], dr[2]);

     rr = Sqr(dr[1]) + Sqr(dr[2]);
     if(rr < rrCut ){
     r = sqrt(rr);
     ri = 1/r;
     uVal = ri*exp(-kappa*r);

     TVal = (1./rr + Sqr(kappa) + kappa/r)*uVal;
     TValSum[i] += TVal;
     TValSum[j] += TVal;
   } }
     AA = Sqr(ax[i]) + Sqr(ay[i]);
     AASum += AA;
     vv = Sqr(vx[i]) + Sqr(vy[i]);
     VVSum += vv;
     deno += TValSum[i];
}

     double gSumconfig, varSconfig, massSconfig;
     if(stepCount == 1) varSconfig = 0.;
     gSumconfig = 0.; massSconfig = 2.0;

     gSumconfig = (AASum/temperature - deno)/massSconfig;
     varSconfig += deltaT*gSumconfig;

      /*****Configarational Nose-Hoover thermostat*****/
   for (n = 1; n <= nAtom; n++){
      vx[n] += deltaT * ax[n];
      rx[n] += deltaT * (vx[n] + varSconfig * ax[n]);
      vy[n] += deltaT * ay[n];
      ry[n] += deltaT * (vy[n] + varSconfig * ay[n]);
    }
      /*****Kinetic Nose-Hoover thermostat*****/
  }else if(thermo == 'N'){
    gSum = (0.5*S2 - (nAtom + 1)*temperature)/massS;
    varS += deltaT*gSum;
   for (n = 1; n <= nAtom; n++){
      vx[n] += deltaT * (ax[n] - varS *vx[n]);
      rx[n] += deltaT * vx[n];
      vy[n] += deltaT * (ay[n] - varS *vy[n]);
      ry[n] += deltaT * vy[n];
   }
      /*****for Gaussian thermostat*****/
 }else if(thermo == 'G'){
      for (n = 1; n <= nAtom; n++){
      vx[n] = C * vx[n] + D * ax[n];
      rx[n] += deltaT * vx[n];
      vy[n] = C * vy[n] + D * ay[n];
      ry[n] += deltaT * vy[n];
     }
   }else if (thermo == 'L'){
  double nu = 0.03066;
  double var = sqrt(2*nu/(GAMMA*deltaT));
  double scale = 1. + nu*deltaT/2.;
  double scale_v = 2./scale - 1.;
  double scale_f = deltaT/scale;
  int n;
  for(n = 1 ; n <= nAtom ; n ++){
      vx[n] = scale_v*vx[n] + scale_f*(ax[n] + var*gsl_ran_gaussian(rnd,1));
      rx[n] += deltaT * vx[n];
      vy[n] = scale_v*vy[n] + scale_f*(ay[n] + var*gsl_ran_gaussian(rnd,1));
      ry[n] += deltaT * vy[n];
    }
  }
 }else{
    int n;
    for(n = 1 ; n <= nAtom ; n ++){
      vx[n] += deltaT * ax[n];
      rx[n] += deltaT * vx[n];
      vy[n] += deltaT * ay[n];
      ry[n] += deltaT * vy[n];
    }
  }
}
```

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

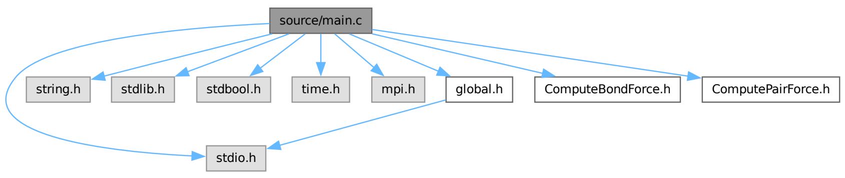
Go to the documentation of this file.

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

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

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


void LeapfrogStep(char thermo, gsl_rng * rnd){
double temperature, GAMMA;
GAMMA = 100;

double *TValSum;
TValSum = (double*)malloc((nAtom + 1) * sizeof(double));


  if(stepCount <= stepEquil){
    double gSum, varS, massS;
    temperature = 1./GAMMA;

   if(stepCount == 1) varS = 0.;
    double A, S1, S2, T;
    int n;
    S1 = 0.; S2 = 0.; gSum = 0.; massS = 0.1;

    vvSum = 0.;
    double halfdt = 0.5*deltaT;
    for (n = 1; n <= nAtom; n++){
      T = vx[n] + halfdt * ax[n];
      S1 += T * ax[n];
      S2 += Sqr(T);

      T = vy[n] + halfdt * ay[n];
      S1 += T * ay[n];
      S2 += Sqr(T);
     vvSum += (Sqr(vx[n]) +  Sqr(vy[n]));
    }

    A = -S1 / S2;
    S2 = vvSum;

    double C = 1 + A*deltaT ;
    double D = deltaT * (1 + 0.5 * A * deltaT);

    int i,j;
    real dr[NDIM+1], r, rr, ri, rrCut;
    double vv;

    double uVal, AA, AASum;
    double TVal;

    double deno, VVSum;
    deno = 0.;
    VVSum = 0.;
    AASum = 0.;

  for(n=1;n<=nAtom; n++)
     TValSum[n] = 0.;

  rrCut = Sqr(rCut);

/*****Calculating Configarational temperature*****/
//Solving the equation of motion here
if(thermo == 'C'){
for(i = 1 ; i <= nAtom; i ++){
    for(j = i+1 ; j <= nAtom ; j ++){
      dr[1] = rx[i] - rx[j];
      if(fabs(dr[1]) > regionH[1])
    dr[1] -= SignR(region[1], dr[1]);

     dr[2] = ry[i] - ry[j];
      if(fabs(dr[2]) > regionH[2])
    dr[2] -= SignR(region[2], dr[2]);

     rr = Sqr(dr[1]) + Sqr(dr[2]);
     if(rr < rrCut ){
     r = sqrt(rr);
     ri = 1/r;
     uVal = ri*exp(-kappa*r);

     TVal = (1./rr + Sqr(kappa) + kappa/r)*uVal;
     TValSum[i] += TVal;
     TValSum[j] += TVal;
   } }
     AA = Sqr(ax[i]) + Sqr(ay[i]);
     AASum += AA;
     vv = Sqr(vx[i]) + Sqr(vy[i]);
     VVSum += vv;
     deno += TValSum[i];
}

     double gSumconfig, varSconfig, massSconfig;
     if(stepCount == 1) varSconfig = 0.;
     gSumconfig = 0.; massSconfig = 2.0;

     gSumconfig = (AASum/temperature - deno)/massSconfig;
     varSconfig += deltaT*gSumconfig;

      /*****Configarational Nose-Hoover thermostat*****/
   for (n = 1; n <= nAtom; n++){
      vx[n] += deltaT * ax[n];
      rx[n] += deltaT * (vx[n] + varSconfig * ax[n]);
      vy[n] += deltaT * ay[n];
      ry[n] += deltaT * (vy[n] + varSconfig * ay[n]);
    }
      /*****Kinetic Nose-Hoover thermostat*****/
  }else if(thermo == 'N'){
    gSum = (0.5*S2 - (nAtom + 1)*temperature)/massS;
    varS += deltaT*gSum;
   for (n = 1; n <= nAtom; n++){
      vx[n] += deltaT * (ax[n] - varS *vx[n]);
      rx[n] += deltaT * vx[n];
      vy[n] += deltaT * (ay[n] - varS *vy[n]);
      ry[n] += deltaT * vy[n];
   }
      /*****for Gaussian thermostat*****/
 }else if(thermo == 'G'){
      for (n = 1; n <= nAtom; n++){
      vx[n] = C * vx[n] + D * ax[n];
      rx[n] += deltaT * vx[n];
      vy[n] = C * vy[n] + D * ay[n];
      ry[n] += deltaT * vy[n];
     }
   }else if (thermo == 'L'){
  double nu = 0.03066;
  double var = sqrt(2*nu/(GAMMA*deltaT));
  double scale = 1. + nu*deltaT/2.;
  double scale_v = 2./scale - 1.;
  double scale_f = deltaT/scale;
  int n;
  for(n = 1 ; n <= nAtom ; n ++){
      vx[n] = scale_v*vx[n] + scale_f*(ax[n] + var*gsl_ran_gaussian(rnd,1));
      rx[n] += deltaT * vx[n];
      vy[n] = scale_v*vy[n] + scale_f*(ay[n] + var*gsl_ran_gaussian(rnd,1));
      ry[n] += deltaT * vy[n];
    }
  }
 }else{
    int n;
    for(n = 1 ; n <= nAtom ; n ++){
      vx[n] += deltaT * ax[n];
      rx[n] += deltaT * vx[n];
      vy[n] += deltaT * ay[n];
      ry[n] += deltaT * vy[n];
    }
  }
}

```

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.

```
                         {
 if(icode == 0){
 sPotEnergy = ssPotEnergy = 0.;
 sKinEnergy = ssKinEnergy = 0.;
 sPressure = ssPressure = 0.;
 sTotEnergy = ssTotEnergy = 0.;
 svirSum = 0.;
 }else if(icode == 1){
 sPotEnergy += potEnergy;
 ssPotEnergy += Sqr(potEnergy);
 sKinEnergy += kinEnergy;
 ssKinEnergy += Sqr(kinEnergy);
 sTotEnergy += totEnergy;
 ssTotEnergy += Sqr(totEnergy);
 sPressure += pressure;
 ssPressure += Sqr(pressure);
 svirSum += virSum;
 }else if(icode == 2){
 sPotEnergy /= stepAvg;
 ssPotEnergy /= sqrt(ssPotEnergy/stepAvg - Sqr(sPotEnergy));
 sTotEnergy /= stepAvg;
 ssTotEnergy = sqrt(ssTotEnergy/stepAvg - Sqr(sTotEnergy));
 sKinEnergy /= stepAvg;
 ssKinEnergy = sqrt(ssKinEnergy/stepAvg - Sqr(sKinEnergy));
 sPressure /= stepAvg;
 ssPressure = sqrt(ssPressure/stepAvg - Sqr(sPressure));
 svirSum /= stepAvg;
 } }
```

3.72.2.2 ApplyBoundaryCond()

```
void ApplyBoundaryCond ( )
```

Definition at line 27 of file ApplyBoundaryCond.c.

```
                        {
  int n;
  for(n = 1 ; n <= nAtom ; n ++){
   if(strcmp(xBoundary, "p") == 0 && strcmp(yBoundary, "p") == 0){          // P.B.C along x and y axis
    rx[n] -= region[1]*rint(rx[n]/region[1]);
    ry[n] -= region[2]*rint(ry[n]/region[2]);
   } else if (strcmp(xBoundary, "r") == 0 && strcmp(yBoundary, "r") == 0){   //R.B.C. along x and y
axis
     if((rx[n] + atomRadius[n]) >= regionH[1]){
        rx[n] = 0.999999*regionH[1] - atomRadius[n]; vx[n] = -vx[n] ;
     }if((rx[n]-atomRadius[n]) < -regionH[1]){
        rx[n] = -0.999999*regionH[1] + atomRadius[n]; vx[n] = -vx[n] ;
    }
     if((ry[n] + atomRadius[n])>= regionH[2]){
        ry[n] = 0.999999*regionH[2] - atomRadius[n]; vy[n] = -vy[n] ;
     }if((ry[n]-atomRadius[n]) < -regionH[2]){
        ry[n] = -0.999999*regionH[2] + atomRadius[n]; vy[n] = -vy[n] ;
    }}
    else if (strcmp(xBoundary, "p") == 0 && strcmp(yBoundary, "r") == 0){   //P.B.C. along x and R.B.C
along y axis
    rx[n] -= region[1]*rint(rx[n]/region[1]);
    if((ry[n] + atomRadius[n]) >= regionH[2]){
      ry[n] = 0.999999*regionH[2] - atomRadius[n]; vy[n] = -vy[n] ;
     }if((ry[n] - atomRadius[n]) < -regionH[2]){
        ry[n] = -0.999999*regionH[2] + atomRadius[n]; vy[n] = -vy[n] ;
  }}
    else if(strcmp(xBoundary, "r") == 0 && strcmp(yBoundary, "p") == 0){   //R.B.C. along x and P.B.C
along y axis
    if((rx[n] + atomRadius[n]) >= regionH[1]){
       rx[n] = 0.999999*regionH[1] - atomRadius[n]; vx[n] = -vx[n] ;
     }if((rx[n] - atomRadius[n]) < -regionH[1]){
      rx[n] = -0.999999*regionH[1] + atomRadius[n]; vx[n] = -vx[n] ;
     }
     ry[n] -= region[2]*rint(ry[n]/region[2]);
  } else {
    // Print error message and exit the program
    fprintf(fpresult, "Error: Invalid boundary configuration: '%s %s'\n", xBoundary, yBoundary);
    exit(EXIT_FAILURE); // Exit with failure status
  }
 }
}
```

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.

```
                            {
 int n;
 double Vxblock, Vyblock;
 double Vxsubstrate, Vysubstrate;
 Vxblock = 0.0;  Vyblock = 0.0;
 Vxsubstrate = 0.0; Vysubstrate = 0.0;
 double gammav;
 gammav = 0.0;

 double count_substrate = 0;
 double count_block = 0;

 for(n = 1 ; n <= nAtom; n ++){
  if(atomType[n] == 1 || atomType[n] == 2){
  Vxsubstrate += vx[n]; Vysubstrate += vy[n];
  count_substrate++;
  }
  if(atomType[n] == 3 || atomType[n] == 4){
  Vxblock += vx[n]; Vyblock += vy[n];
  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 ( )
```

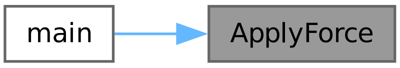
Definition at line 25 of file ApplyForce.c.

```
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;
```

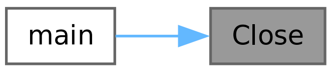
```
      vy[n] = dy/deltaT;
    }
  }
}
```
References ax, ay, deltaT, nAtom, rx, ry, Sqr, stepCount, stepEquil, vx, and vy.

3.72.2.9 Close()

```
void Close ( )
```
Definition at line 24 of file Close.c.
```
                {
  int n;
  free(rx);
  free(ry);
  free(vx);
  free(vy);
  free(ax);
  free(ay);
  free(fax);
  free(fay);
  free(cellList);

  free(atomID); free(atomType); free(atomRadius); free(atomMass);
  free(speed);
  free(atom1); free(atom2); free(BondID);
  free(BondType); free(kb); free(ro);
  free(ImageX); free(ImageY); free(rxUnwrap); free(ryUnwrap);
  free(atomIDInterface);
  free(PairID); free(Pairatom1); free(Pairatom2);
  free(PairXij); free(PairYij);

  free(DeltaXijOld);
  free(DeltaYijOld);

  free(molID);

  for (n = 0; n <= nAtom; n++) {
   free(isBonded[n]);
   }
   free(isBonded);



  for(n = 0; n <= nAtom; n++) {
   free(DeltaXijOldPair[n]);
   free(DeltaYijOldPair[n]);
   }
    free(DeltaXijOldPair);
    free(DeltaYijOldPair);

  for (n = 0; n <= nBuffCorr; n++){
    free(cfOrg[n]);
    free(spacetimeCorr[n]);
  }
  free(cfOrg);
  free(spacetimeCorr);
  free(cfVal);
  free(indexCorr);
  free(spacetimeCorrAv);

  free(indexAcf);
  free(viscAcfOrg);
  free(viscAcfAv);
  for(n = 0 ; n <= nBuffAcf ; n ++)
    free(viscAcf[n]);
  free(viscAcf);

}
```
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];
```

```
          rr = Sqr(dr[1]) + Sqr(dr[2]);
          RadiusIJ = atomRadius[I] + atomRadius[J];
          SqrRadiusIJ = Sqr(RadiusIJ);
          if(rr < SqrRadiusIJ){
        r = sqrt(rr);
        ri = 1.0/r;
                rrinv = 1.0/rr;
                vr[1] = vx[I] - vx[J];
                vr[2] = vy[I] - vy[J];
        RadiusIJInv = 1.0/RadiusIJ;
        uVal = Sqr(1.0 - r * RadiusIJInv);
        fcVal = 2.0 * RadiusIJInv * (1.0 - r * RadiusIJInv) *ri;
                fdVal = -gamman * (vr[1]*dr[1] + vr[2]*dr[2]) * rrinv; //disc-disc drag

        f  = fcVal * dr[1];
                fd = fdVal * dr[1];
        ax[I] += (f + fd);
                discDragx[I] += fd; //disc-disc drag

        f = fcVal * dr[2];
                fd = fdVal * dr[2];
        ay[I] += (f + fd);
                discDragy[I] += fd; //disc-disc drag

        uSum +=  0.5 * uVal;
        virSum += 0.5 * fcVal * rr;
        rfAtom += 0.5 * dr[1] * fcVal * dr[2];
          }
        }else if(m1 != m2 && (atomRadius[I] > 0. && atomRadius[J] > 0.)){
          dr[1] = rx[I] - rx[J] - shift[1];
          dr[2] = ry[I] - ry[J] - shift[2];
          rr = Sqr(dr[1]) + Sqr(dr[2]);
          RadiusIJ = atomRadius[I] + atomRadius[J];
          SqrRadiusIJ = Sqr(RadiusIJ);
          if(rr < SqrRadiusIJ){
        r = sqrt(rr);
        ri = 1.0/r;
                rrinv = 1.0/r;
                vr[1] = vx[I] - vx[J];
                vr[2] = vy[I] - vy[J];
        RadiusIJInv = 1.0/RadiusIJ;
        uVal = Sqr(1.0 - r * RadiusIJInv);
        fcVal = 2.0 * RadiusIJInv * (1.0 - r * RadiusIJInv) *ri;
                fdVal = -gamman * (vr[1]*dr[1] + vr[2]*dr[2]) * rrinv; //disc-disc drag

        f  = fcVal * dr[1];
                fd =  fdVal * dr[1];
        ax[I] += (f + fd);
                discDragx[I] += fd; //disc-disc drag

        f  = fcVal * dr[2];
                fd = fdVal * dr[2];
        ay[I] += (f + fd);
                discDragy[I] += fd; //disc-disc drag

        uSum +=  0.5 * uVal;
        virSum += 0.5 * fcVal * rr;
        rfAtom += 0.5 * dr[1] * fcVal * dr[2];
          }
        }
            J = cellList[J];
      }
      I = cellList[I];
    }
      }
    }
  }
}
```

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()

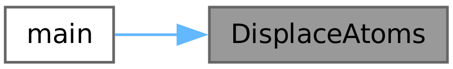
```
void DisplaceAtoms ( )
```

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:



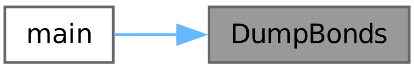
3.72.2.12 DumpBonds()

```
void DumpBonds ( )
```

Definition at line 24 of file DumpBonds.c.

```
                  {
  int n;
  //Trajectory file in LAMMPS dump format for OVITO visualization
  fprintf(fpbond, "ITEM: TIMESTEP\n");
  fprintf(fpbond, "%lf\n",timeNow);
  fprintf(fpbond, "ITEM: NUMBER OF ENTRIES\n");
  fprintf(fpbond, "%d\n",nBond);
  fprintf(fpbond, "ITEM: BOX BOUNDS pp ff pp\n");
  fprintf(fpbond, "%lf %lf xlo xhi\n", -regionH[1], regionH[1]);
  fprintf(fpbond, "%lf %lf ylo yhi\n", -regionH[2], regionH[2]);
  fprintf(fpbond, "%lf %lf zlo zhi\n", -0.1, 0.1);
  fprintf(fpbond, "ITEM: ENTRIES BondID, BondType, atom1 atom2 BondLength BondLengthEqul nodeDragx1
nodeDragy1\n");

  for(n=1; n<=nBond; n++)
   fprintf(fpbond, "%d %d %d %d %0.16lf %0.16lf %0.16lf %0.16lf\n", BondID[n], BondType[n], atom1[n],
atom2[n],
   BondLength[n], ro[n], nodeDragx[atom1[n]], nodeDragy[atom1[n]]);
  }
```

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 ( )
```

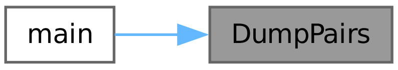
Definition at line 25 of file DumpPairs.c.

```
                  {
  int n;
  //Trajectory file in LAMMPS dump format for OVITO visualization
  fprintf(fppair, "ITEM: TIMESTEP\n");
  fprintf(fppair, "%lf\n",timeNow);
  fprintf(fppair, "ITEM: NUMBER OF ENTRIES\n");
  fprintf(fppair, "%d\n",nPairActive);
  fprintf(fppair, "ITEM: BOX BOUNDS pp ff pp\n");
  fprintf(fppair, "%lf %lf xlo xhi\n", -regionH[1], regionH[1]);
  fprintf(fppair, "%lf %lf ylo yhi\n", -regionH[2], regionH[2]);
  fprintf(fppair, "%lf %lf zlo zhi\n", -0.1, 0.1);
  fprintf(fppair, "ITEM: ENTRIES index, atom1 atom2 xij yij discDragx1 discDragy1\n");

  for(n=1; n<=nPairActive; n++)
   fprintf(fppair, "%d %d %d %0.16lf %0.16lf %0.16lf %0.16lf\n", PairID[n], Pairatom1[n],
      Pairatom2[n],
   PairXij[n], PairYij[n], discDragx[n], discDragy[n]);

  }
```

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 ( )
```

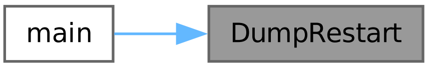
Definition at line 25 of file DumpRestart.c.

```
                   {
 char DUMP[256];
 FILE *fpDUMP;
 sprintf(DUMP, "%s.Restart", prefix);
 fpDUMP = fopen(DUMP, "w");
 if(fpDUMP == NULL) {
  fprintf(stderr, "Error opening file %s for writing\n", DUMP);
  return;
 }

  fprintf(fpDUMP, "timeNow %lf\n", timeNow);
  fprintf(fpDUMP, "nAtom %d\n",  nAtom);
  fprintf(fpDUMP, "nBond %d\n", nBond);
  fprintf(fpDUMP, "nAtomType %d\n", nAtomType);
  fprintf(fpDUMP, "nBondType %d\n", nBondType);
  fprintf(fpDUMP, "region[1] %0.14lf\n", region[1]);
  fprintf(fpDUMP, "region[2] %0.14lf\n", region[2]);

  int n;
  fprintf(fpDUMP, "Atoms\n");
  for(n = 1; n <= nAtom; n ++)
   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]);


  fprintf(fpDUMP, "Bonds\n");
  for(n=1; n<=nBond; n++)
  fprintf(fpDUMP,  "%d %d %d %d %0.2lf %0.16lf\n", BondID[n], BondType[n], atom1[n], atom2[n], kb[n],
      ro[n]);

  fclose(fpDUMP);
 }
```

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 ( )
```

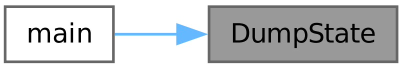
Definition at line 25 of file DumpState.c.

```
                         {
 char DUMP[256];
 FILE *fpDUMP;
 sprintf(DUMP, "%s.STATE", prefix);
 fpDUMP = fopen(DUMP, "w");
 if(fpDUMP == NULL) {
  fprintf(stderr, "Error opening file %s for writing\n", DUMP);
  return;
 }

  fprintf(fpDUMP, "ITEM: TIMESTEP\n");
  fprintf(fpDUMP, "%lf\n",timeNow);
  fprintf(fpDUMP, "ITEM: NUMBER OF ATOMS\n");
  fprintf(fpDUMP, "%d\n",nAtom);
  fprintf(fpDUMP, "ITEM: BOX BOUNDS pp pp pp\n");
  fprintf(fpDUMP, "%lf %lf xlo xhi\n", -regionH[1], regionH[1]);
  fprintf(fpDUMP, "%lf %lf ylo yhi\n", -regionH[2], regionH[2]);
  fprintf(fpDUMP, "%lf %lf zlo zhi\n",  -0.1, 0.1);
  fprintf(fpDUMP, "ITEM: ATOMS id mol type radius x y vx vy fx fy\n");
  int n;
  for (n = 1; n <= nAtom; n++) {
   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",
   atomID[n], molID[n], atomType[n], atomRadius[n], rx[n], ry[n], vx[n], vy[n], ax[n], ay[n]);
  }
  fclose(fpDUMP);
}
```

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.

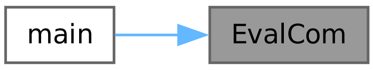
```
               {
 int n;
 ComX = 0.0; ComY = 0.0; ComXRatio = 0.0; ComYRatio = 0.0;
 TotalMass = 0.0;

 for(n=1; n<=nAtom; n++){
```

```
 if(molID[n] == 2){
  ComX += atomMass[n] * rxUnwrap[n];
  ComY += atomMass[n] * ryUnwrap[n];
  TotalMass += atomMass[n];
  } }

  ComX = ComX/TotalMass;
  ComY = ComY/TotalMass;

  if(timeNow == 0.0){
  ComX0 = ComX; ComY0 = ComY;
  }
  ComXRatio = ComX/ComX0;    ComYRatio = ComY/ComY0;
 }
```

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 ( )
```

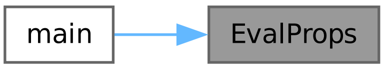
Definition at line 26 of file EvalProps.c.

```
                      {
 real v, vv;
 virSum = 0.0;
 vSumX = 0.0; vSumY = 0.0; vSum = 0.0;
 vvSum = 0.;
 int n;

 for (n = 1; n <= nAtom; n++) {
  vv = 0.;
  // Initialize v with a default value to avoid "uninitialized" warning.
  v = 0.0;
  // X direction velocity
  if (strcmp(solver, "Verlet") == 0) {
    v = vx[n];
  } else if (strcmp(solver, "LeapFrog") == 0) {
    v = vx[n] - 0.5 * deltaT * ax[n];
  }
   vSum += v;
   vv += Sqr(v);
   vSumX += v;
   // Y direction velocity
   if (strcmp(solver, "Verlet") == 0) {
   v = vy[n];
   } else if (strcmp(solver, "LeapFrog") == 0) {
   v = vy[n] - 0.5 * deltaT * ay[n];
   }
   vSum += v;
   vSumY += v;
   vv += Sqr(v);
   vvSum += vv;
  }

  kinEnergy = 0.5 * vvSum / nAtom ;
  uSumPairPerAtom = uSumPair / nAtom ;
  BondEnergyPerAtom = TotalBondEnergy / (0.5*nAtom); //Factor of 0.5 since each atom has one half the
bond energy
  potEnergy = uSumPairPerAtom +  BondEnergyPerAtom ;
  totEnergy = kinEnergy + potEnergy;
  virSumxx = virSumPairxx  + virSumBondxx ;
  virSumyy = virSumPairyy  + virSumBondyy ;
  virSumxy = virSumPairxy  + virSumBondxy ;
  virSum = virSumPair + virSumBond;
  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++){
    tVal = (n-1)*stepCorr*deltaT;
    fprintf (fpdnsty, "%e\t", tVal);
    int nn = nFunCorr*(n-1);
    for (j = 1; j <= nFunCorr; j ++)
         fprintf (fpdnsty, "%e\t", spacetimeCorrAv[nn + j]);
       fprintf (fpdnsty, "\n");
     }

     countCorrAv = 0.;
     for (j = 1; j <= nFunCorr*nValCorr; j++)
    spacetimeCorrAv[j] = 0.;
    }
  }
 }
}
```

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

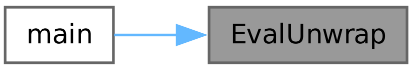
3.72.2.20 EvalUnwrap()

```
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()

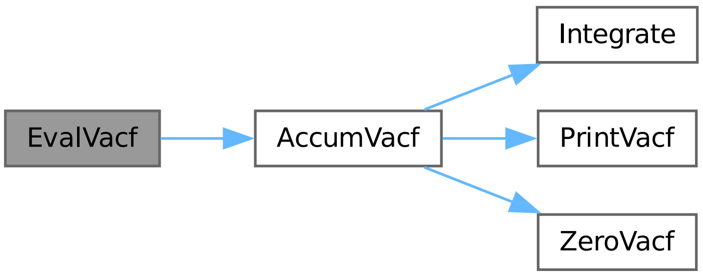
```
void EvalVacf ( )
```

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 ( )
```

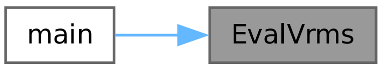
Definition at line 27 of file EvalVrms.c.

```
                    {
   int n;
   VSqr = 0.0;
   VMeanSqr = 0.0;
   VRootMeanSqr = 0.0;

   for(n = 1 ; n <= nAtom ; n ++){
   VSqr += Sqr(vx[n]) + Sqr(vy[n]);
   }
   VMeanSqr = VSqr/nAtom;
   VRootMeanSqr = sqrt(VMeanSqr);
   }
```

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.

```
                                                 {

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

References fpresult, HaltCondition, and stepCount.
Referenced by main().
Here is the caller graph for this function:

main
HaltConditionCheck

3.72.2.24 Init()

`void Init ( )`

Definition at line 29 of file Init.c.

```
          {
  char dummy[128];
  char inputConfig[128];
  FILE *fp;
  fp = fopen("input-data","r");
  fscanf(fp, "%s %s", dummy, inputConfig);
  fscanf(fp, "%s %s", dummy, solver);
  fscanf(fp, "%s %s %s", dummy, xBoundary, yBoundary);
  fscanf(fp, "%s %d",  dummy, &DampFlag);
  fscanf(fp, "%s %d",  dummy, &freezeAtomType);
  fscanf(fp, "%s %lf", dummy, &rCut);
  fscanf(fp, "%s %lf", dummy, &gamman);
  fscanf(fp, "%s %lf", dummy, &kappa);
  fscanf(fp, "%s %lf", dummy, &deltaT);
  fscanf(fp, "%s %lf", dummy, &strain);
  fscanf(fp, "%s %lf", dummy, &FyBylx);
  fscanf(fp, "%s %lf", dummy, &fxByfy);
  fscanf(fp, "%s %lf", dummy, &DeltaY);
  fscanf(fp, "%s %lf", dummy, &DeltaX);
  fscanf(fp, "%s %lf", dummy, &HaltCondition);
  fscanf(fp, "%s %d",  dummy, &stepAvg);
  fscanf(fp, "%s %d",  dummy, &stepEquil);
  fscanf(fp, "%s %d",  dummy, &stepLimit);
  fscanf(fp, "%s %d",  dummy, &stepDump);
  fscanf(fp, "%s %d",  dummy, &stepTraj);
  fscanf(fp, "%s %d",  dummy, &limitCorrAv);
  fscanf(fp, "%s %d",  dummy, &nBuffCorr);
  fscanf(fp, "%s %d",  dummy, &nFunCorr);
  fscanf(fp, "%s %d",  dummy, &nValCorr);
  fscanf(fp, "%s %d",  dummy, &stepCorr);
  fscanf(fp, "%s %d",  dummy, &limitAcfAv);
  fscanf(fp, "%s %d",  dummy, &nBuffAcf);
  fscanf(fp, "%s %d",  dummy, &nValAcf);
  fscanf(fp, "%s %d",  dummy, &stepAcf);
  fscanf(fp, "%s %lf", dummy, &rangeRdf);
  fscanf(fp, "%s %d",  dummy, &limitRdf);
  fscanf(fp, "%s %d",  dummy, &sizeHistRdf);
  fscanf(fp, "%s %d",  dummy, &stepRdf);

  fclose(fp);
  FILE *fpSTATE;
  if((fpSTATE = fopen(inputConfig,"r"))==NULL){
  printf("Error occurred: Could not open STATE file\n Exiting now..\n");
  exit(0);
  }

  fscanf(fpSTATE, "%s %lf", dummy, &timeNow);
  fscanf(fpSTATE, "%s %d",  dummy, &nAtom);
  fscanf(fpSTATE, "%s %d",  dummy, &nBond);
  fscanf(fpSTATE, "%s %d",  dummy, &nAtomType);
  fscanf(fpSTATE, "%s %d",  dummy, &nBondType);
  fscanf(fpSTATE, "%s %lf", dummy, &region[1]);
  fscanf(fpSTATE, "%s %lf", dummy, &region[2]);

  region[2] *= 1.5; //Remove this when put on GitHub

  density = nAtom/(region[1]*region[2]);
  cells[1] = region[1] / rCut;
  cells[2] = region[2] / rCut;
```

```c
  cellList = (int*)malloc((nAtom + cells[1] * cells[2] + 1) * sizeof(int));
  regionH[1] = 0.5*region[1];
  regionH[2] = 0.5*region[2];

  //strain information
  strainRate = strain/deltaT;
  shearDisplacement = strain * region[2];
  shearVelocity = strainRate * region[2];
  int n;

  rx = (double*)malloc((nAtom + 1) * sizeof(double));
  ry = (double*)malloc((nAtom + 1) * sizeof(double));
  vx = (double*)malloc((nAtom + 1) * sizeof(double));
  vy = (double*)malloc((nAtom + 1) * sizeof(double));
  ax = (double*)malloc((nAtom + 1) * sizeof(double));
  ay = (double*)malloc((nAtom + 1) * sizeof(double));
  fax = (double*)malloc((nAtom + 1) * sizeof(double));
  fay = (double*)malloc((nAtom + 1) * sizeof(double));
  atomID = (int*)malloc((nAtom+1) * sizeof(int));
  atomType = (int*)malloc((nAtom+1) * sizeof(int));
  atomRadius = (double*)malloc((nAtom + 1) * sizeof(double));
  atomMass = (double*)malloc((nAtom + 1) * sizeof(double));
  speed = (double*)malloc((nAtom + 1) * sizeof(double));
  atom1 = (int*)malloc((nBond+1)*sizeof(int));
  atom2 = (int*)malloc((nBond+1)*sizeof(int));
  BondID = (int*)malloc((nBond+1)*sizeof(int));
  BondType = (int*)malloc((nBond+1)*sizeof(int));
  kb = (double*)malloc((nBond+1)*sizeof(double));
  ro = (double*)malloc((nBond+1)*sizeof(double));
  BondEnergy = (double*)malloc((nBond+1)*sizeof(double));
  BondLength =(double*)malloc((nBond+1)*sizeof(double));
  discDragx = (double*)malloc((nAtom + 1) * sizeof(double));
  discDragy = (double*)malloc((nAtom + 1) * sizeof(double));
  nodeDragx = (double*)malloc((nAtom + 1) * sizeof(double));
  nodeDragy = (double*)malloc((nAtom + 1) * sizeof(double));
  ImageX = (int*)malloc((nAtom+1) * sizeof(int));
  ImageY = (int*)malloc((nAtom+1) * sizeof(int));
  rxUnwrap = (double*)malloc((nAtom + 1) * sizeof(double));
  ryUnwrap = (double*)malloc((nAtom + 1) * sizeof(double));
  DeltaXijOld = (double*)malloc((nBond+1)*sizeof(double));
  DeltaYijOld = (double*)malloc((nBond+1)*sizeof(double));
  DeltaXijOldPair = (double**)malloc((nAtom+1) * sizeof(double*));
  DeltaYijOldPair = (double**)malloc((nAtom+1) * sizeof(double*));
  for(int n = 0; n <= nAtom; n++) {
   DeltaXijOldPair[n] = (double*)malloc((nAtom+1) * sizeof(double));
   DeltaYijOldPair[n] = (double*)malloc((nAtom+1) * sizeof(double));
  }
  molID = (int*)malloc((nAtom+1) * sizeof(int));

  for(n = 1; n <= nAtom; n ++){
   atomMass[n] = 1.0;
  }

  fscanf(fpSTATE, "%s\n", dummy);
  for(n = 1; n <= nAtom; n ++)
   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]);


  fscanf(fpSTATE, "%s\n", dummy);
  for(n=1; n<=nBond; n++)
   fscanf(fpSTATE, "%d %d %d %d %lf %lf\n", &BondID[n], &BondType[n], &atom1[n], &atom2[n], &kb[n], &ro[n]);

  fclose(fpSTATE);

 //2D-List of bonded atoms. This is used to remove pair interaction
 //calculation for the bonded atoms
   isBonded = (int**)malloc((nAtom + 1) * sizeof(int*));
  for (int i = 0; i <= nAtom; i++) {
    isBonded[i] = (int*)malloc((nAtom + 1) * sizeof(int));
    for (int j = 0; j <= nAtom; j++) {
        isBonded[i][j] = 0;
    }
  }

  for (n = 1; n <= nBond; n++) {
    int i = atom1[n];
    int j = atom2[n];
    isBonded[i][j] = 1;
    isBonded[j][i] = 1; // symmetric
}

 //For thermostate, update in final version
thermo = 'C';


```

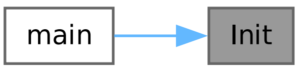
```
// List the interface atoms
nAtomInterface = 0;
nAtomBlock = 0;
nDiscInterface = 0;
double InterfaceWidth, bigDiameter;
bigDiameter = 2.8;
InterfaceWidth = 5.0 * bigDiameter;

for(n = 1; n <= nAtom; n++){
 if(fabs(ry[n]) < InterfaceWidth){
 nAtomInterface++;
 }
 if(molID[n] == 2){
 nAtomBlock++;
 }
 if(atomRadius[n] != 0.0){
 nDiscInterface++;
 } }

  atomIDInterface =  (int*)malloc((nAtomInterface+1)*sizeof(int));

 int m;
 m = 1;
 for(n=1; n<=nAtom; n++){
  if(fabs(ry[n]) < InterfaceWidth){
  atomIDInterface[m] = atomID[n];
  m++;
  } }

 nPairTotal = 0.5 * nAtomInterface * (nAtomInterface-1);
 PairID = (int*)malloc((nPairTotal+1) * sizeof(int));
 Pairatom1 = (int*)malloc((nPairTotal+1) * sizeof(int));
 Pairatom2 = (int*)malloc((nPairTotal+1) * sizeof(int));
 PairXij = (double*)malloc((nPairTotal+1) * sizeof(double));
 PairYij = (double*)malloc((nPairTotal+1) * sizeof(double));

   fprintf(fpresult, "------------------------------------\n");
   fprintf(fpresult, "-------PARAMETERS-----------\n");
   fprintf(fpresult, "------------------------------------\n");
   fprintf(fpresult, "nAtom\t\t\t%d\n",  nAtom);
   fprintf(fpresult, "nBond\t\t\t%d\n",  nBond);
   fprintf(fpresult, "nAtomBlock\t\t%d\n",  nAtomBlock);
   fprintf(fpresult, "nAtomInterface\t%d\n",  nAtomInterface);
   fprintf(fpresult, "nDiscInterface\t\t%d\n",  nDiscInterface);
   fprintf(fpresult, "gamman\t\t\t%0.6g\n", gamman);
   fprintf(fpresult, "strain\t\t\t%0.6g\n", strain);
   fprintf(fpresult, "strainRate\t\t%0.6g\n", strainRate);
   fprintf(fpresult, "FyBylx\t\t\t%0.6g\n", FyBylx);
   fprintf(fpresult, "fxByfy\t\t\t%0.6g\n", fxByfy);
   fprintf(fpresult, "DeltaY\t\t\t%0.6g\n", DeltaY);
   fprintf(fpresult, "DeltaX\t\t\t%0.6g\n", DeltaX);
   fprintf(fpresult, "HaltCondition\t\t%0.6g\n", HaltCondition);
   fprintf(fpresult, "kappa\t\t\t%g\n", kappa);
   fprintf(fpresult, "density\t\t\t%g\n", density);
   fprintf(fpresult, "rCut\t\t\t\t%g\n", rCut);
   fprintf(fpresult, "deltaT\t\t\t%g\n", deltaT);
   fprintf(fpresult, "stepEquil\t\t\t%d\n",  stepEquil);
   fprintf(fpresult, "stepLimit\t\t\t%d\n",  stepLimit);
   fprintf(fpresult, "region[1]\t\t\t%0.16lf\n", region[1]);
   fprintf(fpresult, "region[2]\t\t\t%0.16lf\n", region[2]);
   fprintf(fpresult, "cells[1]\t\t\t%d\n",  cells[1]);
   fprintf(fpresult, "cells[2]\t\t\t%d\n",  cells[2]);
   fprintf(fpresult, "solver\t\t\t%s\n",  solver);
   fprintf(fpresult, "boundary\t\t\t%s %s\n", xBoundary, yBoundary);
   fprintf(fpresult, "DampFlag\t\t%d\n",  DampFlag);


   fprintf(fpresult, "------------------------------------\n");
   fprintf(fpresult, "#TimeNow TotalMomentum PotEngyPerAtom KinEngyPerAtom TotEngyPerAtom
PairEnergyPerAtom BondEnergyPerAtom  Press VirialSum\n");
   fprintf(fpvrms, "#timeNow\tVrms \n");
   fprintf(fpcom, "#timeNow\tComX\tComY\n");

/* //Uncomment the following as per your acquirement
   fprintf(fpstress, "strain           %lf\n", strain);
   fprintf(fpstress, "region[1]        %lf\n", region[1]);
   fprintf(fpstress, "region[2]        %lf\n", region[2]);
   fprintf(fpstress, "#timeNow virSumxx virSumyy virSumxy pressure\n");
   fprintf(fpmomentum, "#timeNow Px Py\n");
*/

  if((strcmp(xBoundary, "p") != 0 && strcmp(xBoundary, "r") != 0) ||
   (strcmp(yBoundary, "p") != 0 && strcmp(yBoundary, "r") != 0)) {
   fprintf(fpresult, "Error: Invalid boundary value detected: '%s %s'. Only 'p' or 'r' are
allowed.\n", xBoundary, yBoundary);
   exit(EXIT_FAILURE); // Exit with failure status
 }
```

```
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 )
```

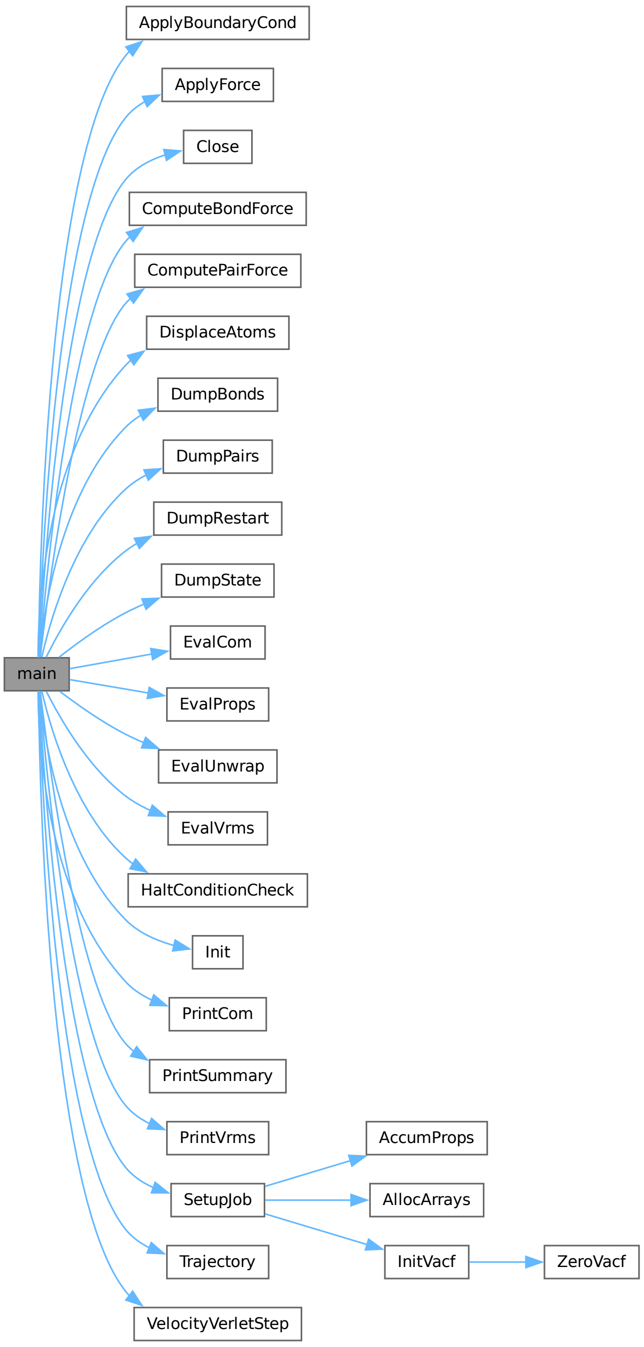
Definition at line 51 of file main.c.

```
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);
```

```
  fpstress = fopen(stress, "w");
  sprintf(momentum, "%s.momentum", prefix);
  fpmomentum = fopen(momentum, "w");
  */

  Init();
  SetupJob();
  t1 = time(NULL);
  moreCycles = 1;
  timeNow = 0.0;
  if(timeNow == 0.0) {
   DisplaceAtoms();
   ComputePairForce(1);
   ComputeBondForce();
   ApplyForce();
   DumpBonds();
   DumpPairs();
   Trajectory();
   EvalUnwrap();
   ApplyBoundaryCond();
   EvalProps();
   EvalVrms();
   EvalCom();
   PrintVrms();
   PrintCom();
   PrintSummary();
   }

//Here starts the main loop of the program
  while(moreCycles){
   if(stepLimit == 0){
   exit(0);
   }

   stepCount ++;
   timeNow = stepCount * deltaT; //for adaptive step size: timeNow += deltaT

   VelocityVerletStep(1);
   EvalUnwrap();
   ApplyBoundaryCond();
   ComputePairForce(1);
   ComputeBondForce();
   ApplyForce();
   VelocityVerletStep(2);
   ApplyBoundaryCond();
   EvalProps();
   EvalVrms();
   EvalCom();
   if(stepCount % stepAvg == 0){
    PrintSummary();
    PrintVrms();
    PrintCom();
    }
   if(stepCount % stepTraj == 0){
    Trajectory();
    DumpBonds();
    DumpPairs();
    }
   if(stepCount % stepDump == 0){
    DumpRestart();      // Save the current state for input
    DumpState();        // Save the current state for config
   }
   if(HaltConditionCheck(VRootMeanSqr, stepCount)) {
    DumpRestart();      // Save the current state for input
    DumpState();        // Save the current state for config
    break;  // Exit the loop when the halt condition is met
    }

    if(stepCount >= stepLimit)
     moreCycles = 0;
  }


  t2 = time(NULL);
  fprintf(fpresult, "#Execution time %lf secs\n", difftime(t2,t1));
  fprintf(fpresult, "#Execution speed %lf steps per secs\n", stepLimit/difftime(t2,t1));

  fclose(fpresult);
  fclose(fpxyz);
  fclose(fpvrms);
  fclose(fpbond);
  fclose(fppair);
  fclose(fpcom);

/*//Uncomment the following as per your acquirement
  fclose(fpdnsty);
  fclose(fpvisc);
  fclose(fprdf);
  fclose(fpstress);
  fclose(fpmomentum);
*/

  free(prefix);
  Close();
  return 0;
}
```

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()

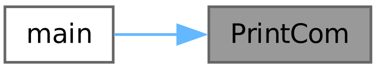
```
void PrintCom ( )
```

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.

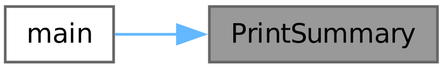
3.72.2.30 PrintSummary()

```
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\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 ( )
```

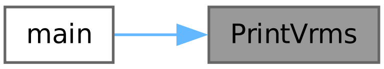
Definition at line 27 of file PrintVrms.c.

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

References fpvrms, timeNow, and VRootMeanSqr.

Referenced by main().

Here is the caller graph for this function:



3.72.2.32 SetupJob()

```
void SetupJob ( )
```

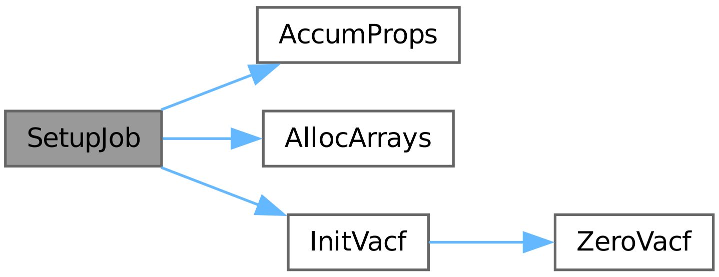
Definition at line 27 of file SetupJob.c.

```
{
  AllocArrays();
  AccumProps(0);
  InitVacf();
  stepCount = 0;
  // INITIALISE SPACETIME CORRELATIONS
  int n;
  for (n = 1; n <= nBuffCorr; n++)
    indexCorr[n] = -(n - 1)*nValCorr/nBuffCorr;

  countCorrAv = 0.;

  for (n = 1; n <= nFunCorr*nValCorr; n++)
    spacetimeCorrAv[n] = 0.;

  //RDF
  countRdf = 0;
}
```

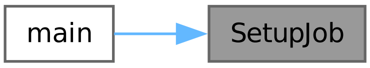
References AccumProps(), AllocArrays(), countCorrAv, countRdf, indexCorr, InitVacf(), nBuffCorr, nFunCorr, nValCorr, spacetimeCorrAv, and stepCount.

Referenced by main().

Here is the call graph for this function:



Here is the caller graph for this function:



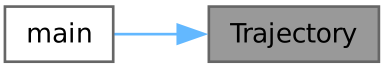
3.72.2.33 Trajectory()

```
void Trajectory ( )
```

Definition at line 25 of file Trajectory.c.

```
                  {
 int n;
 //Trajectory file in LAMMPS dump format for OVITO visualization
 fprintf(fpxyz, "ITEM: TIMESTEP\n");
 fprintf(fpxyz, "%lf\n",timeNow);
 fprintf(fpxyz, "ITEM: NUMBER OF ATOMS\n");
 fprintf(fpxyz, "%d\n",nAtom);
 fprintf(fpxyz, "ITEM: BOX BOUNDS pp ff pp\n");
 fprintf(fpxyz, "%lf %lf xlo xhi\n", -regionH[1], regionH[1]);
 fprintf(fpxyz, "%lf %lf ylo yhi\n", -regionH[2], regionH[2]);
 fprintf(fpxyz, "%lf %lf zlo zhi\n", -0.1, 0.1);
 fprintf(fpxyz, "ITEM: ATOMS id mol type radius x y vx vy fx fy\n");
 for(n=1; n<=nAtom; n++)
  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",
  atomID[n], molID[n], atomType[n], atomRadius[n], rx[n], ry[n], vx[n], vy[n], ax[n], ay[n]);
}
```

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.

```
                                    {
int n;
 if(icode == 1){
 for (n= 1; n <= nAtom; n++) {
  if(atomType[n] != freezeAtomType){
  vx[n] += ax[n] * 0.5 * deltaT;
  vy[n] += ay[n] * 0.5 * deltaT;
  rx[n] += vx[n] * deltaT;
  ry[n] += vy[n] * deltaT;
  }
  //Calculating the image flags here
  if (rx[n] >= regionH[1]) {
   rx[n] -= region[1];
   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:

main
VelocityVerletStep

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();
```

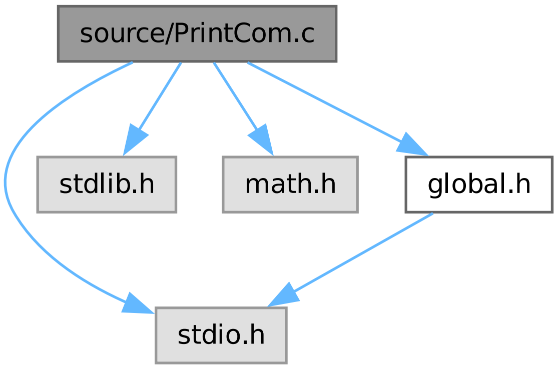
```
void DumpBonds();
void VelocityVerletStep(int icode);
void ApplyForce();
void ApplyDrivingForce();
void ApplyShear();
void ApplyLeesEdwardsBoundaryCond();
void PrintStress();
void Close();
//void ComputePairForce(int normFlag);
void PrintMomentum();
void DisplaceAtoms();
void DumpRestart();
bool HaltConditionCheck(double value, int stepCount);
void EvalCom();
void PrintCom();
void EvalVrms();
void EvalUnwrap();
void DumpPairs();
void ApplyViscous();

int main(int argc, char **argv) {
 time_t t1 = 0, t2;
 if (argc < 2) {
 fprintf(stderr, "Usage: %s <output_prefix>\n", argv[0]);
 return 1;
 }
  int prefix_size = snprintf(NULL, 0, "../output/%s", argv[1]) + 1; // +1 for the null terminator
  prefix = malloc(prefix_size);
  if(prefix == NULL) {
   fprintf(stderr, "Memory allocation failed\n");
   return 1;
   }

   // Write the formatted string into the allocated space
  snprintf(prefix, prefix_size, "../output/%s", argv[1]);
  sprintf(result, "%s.result", prefix);
  fpresult = fopen(result, "w");
  sprintf(xyz, "%s.xyz", prefix);
  fpxyz = fopen(xyz, "w");
  sprintf(vrms, "%s.vrms", prefix);
  fpvrms = fopen(vrms, "w");
  sprintf(bond, "%s.bond", prefix);
  fpbond = fopen(bond, "w");
  sprintf(com, "%s.com", prefix);
  fpcom = fopen(com, "w");
  sprintf(pair, "%s.pair", prefix);
  fppair = fopen(pair, "w");

  /* //Uncomment the following as per your acquirement
  sprintf(dnsty, "%s.curr-dnsty", prefix);
  fpdnsty = fopen(dnsty, "w");
  sprintf(visc, "%s.viscosity", prefix);
  fpvisc = fopen(visc, "w");
  sprintf(rdf, "%s.rdf", prefix);
  fprdf = fopen(rdf, "w");
  sprintf(stress, "%s.stress", prefix);
  fpstress = fopen(stress, "w");
  sprintf(momentum, "%s.momentum", prefix);
  fpmomentum = fopen(momentum, "w");
  */

  Init();
  SetupJob();
  t1 = time(NULL);
  moreCycles = 1;
  timeNow = 0.0;
  if(timeNow == 0.0) {
   DisplaceAtoms();
   ComputePairForce(1);
   ComputeBondForce();
   ApplyForce();
   DumpBonds();
   DumpPairs();
   Trajectory();
   EvalUnwrap();
   ApplyBoundaryCond();
   EvalProps();
   EvalVrms();
   EvalCom();
   PrintVrms();
   PrintCom();
   PrintSummary();
   }

//Here starts the main loop of the program
  while(moreCycles){
   if(stepLimit == 0){
```

```
   exit(0);
   }

   stepCount ++;
   timeNow = stepCount * deltaT; //for adaptive step size: timeNow += deltaT

   VelocityVerletStep(1);
   EvalUnwrap();
   ApplyBoundaryCond();
   ComputePairForce(1);
   ComputeBondForce();
   ApplyForce();
   VelocityVerletStep(2);
   ApplyBoundaryCond();
   EvalProps();
   EvalVrms();
   EvalCom();
   if(stepCount % stepAvg == 0){
    PrintSummary();
    PrintVrms();
    PrintCom();
    }
   if(stepCount % stepTraj == 0){
    Trajectory();
    DumpBonds();
    DumpPairs();
    }
   if(stepCount % stepDump == 0){
    DumpRestart();     // Save the current state for input
    DumpState();       // Save the current state for config
   }
   if(HaltConditionCheck(VRootMeanSqr, stepCount)) {
    DumpRestart();     // Save the current state for input
    DumpState();       // Save the current state for config
    break;  // Exit the loop when the halt condition is met
    }

    if(stepCount >= stepLimit)
     moreCycles = 0;
  }


  t2 = time(NULL);
  fprintf(fpresult, "#Execution time %lf secs\n", difftime(t2,t1));
  fprintf(fpresult, "#Execution speed %lf steps per secs\n", stepLimit/difftime(t2,t1));

  fclose(fpresult);
  fclose(fpxyz);
  fclose(fpvrms);
  fclose(fpbond);
  fclose(fppair);
  fclose(fpcom);

/*//Uncomment the following as per your acquirement
  fclose(fpdnsty);
  fclose(fpvisc);
  fclose(fprdf);
  fclose(fpstress);
  fclose(fpmomentum);
*/

  free(prefix);
  Close();
  return 0;
}
```

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 ( )
```

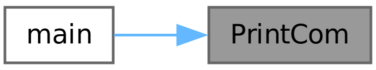
Definition at line 28 of file PrintCom.c.

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

References ComX, ComY, fpcom, and timeNow.

Referenced by main().

Here is the caller graph for this function:



3.75 PrintCom.c

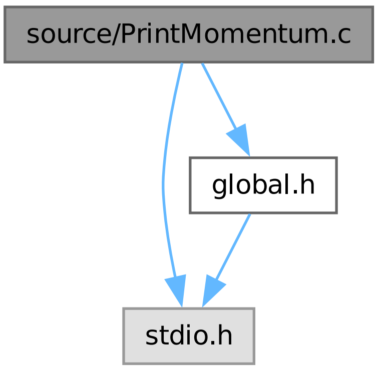
Go to the documentation of this file.

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

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

 */



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

void PrintCom(){
 fprintf(fpcom, "%0.4lf\t%0.16lf\t%0.16lf\n", timeNow, ComX, ComY);
 fflush(fpcom);
 }



```

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

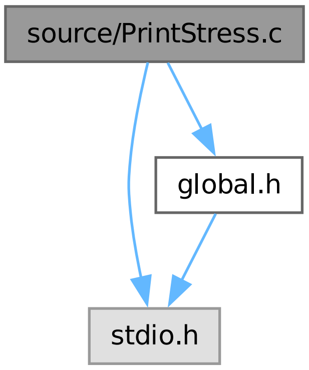
Go to the documentation of this file.

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

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

 */


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

void PrintMomentum(){
 fprintf(fpmomentum, "%0.4lf\t%0.16lf\t%0.16lf\n", timeNow, vSumX, vSumY);
 fflush(fpmomentum);
}
```

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.

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

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

3.79 PrintStress.c

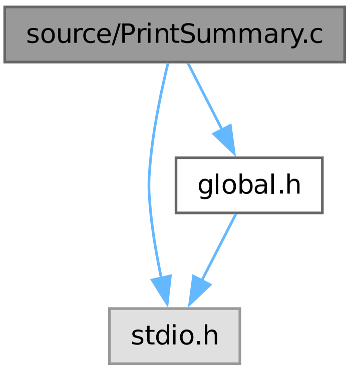
Go to the documentation of this file.

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

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

 */


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

void PrintStress(){
  fprintf(fpstress, "%0.4lf\t%0.16lf\t%0.16lf\t%0.16lf\t%0.16lf\n", timeNow, virSumxx, virSumyy,
     virSumxy, pressure);
  fflush(fpstress);
}
```

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 ( )
```

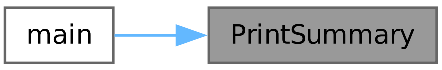
Definition at line 4 of file PrintSummary.c.

```
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\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

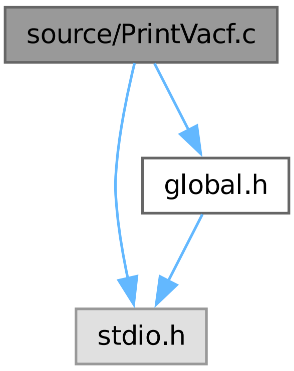
Go to the documentation of this file.

```
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 ( )
```

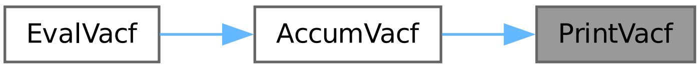
Definition at line 25 of file PrintVacf.c.

```
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.

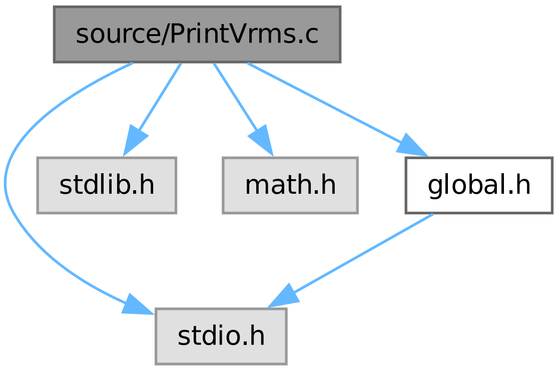
```
00001 /*
00002  * This file is part of Lamina.
00003  *
```

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

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

 */


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

void PrintVacf(){
 double tVal;
 int j;
 fprintf(fpvisc,"viscosity acf\n");
 for(j = 1 ; j <= nValAcf ; j ++){
  tVal = (j-1)*stepAcf*deltaT;
  fprintf(fpvisc, "%lf\t %lf\t %lf\n", tVal, viscAcfAv[j], viscAcfAv[j]/viscAcfAv[1]);
  }
 fprintf(fpvisc, "viscosity acf integral : %lf\n", viscAcfInt);
}


```

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 ( )
```

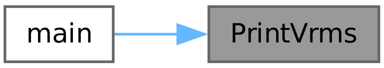
Definition at line 27 of file PrintVrms.c.

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

References fpvrms, timeNow, and VRootMeanSqr.

Referenced by main().

Here is the caller graph for this function:



3.85 PrintVrms.c

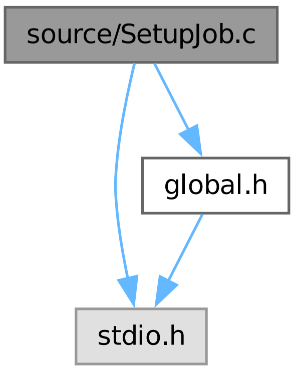
Go to the documentation of this file.

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

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

 */


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

void PrintVrms(){
 fprintf(fpvrms, "%0.4lf\t%0.16lf\n", timeNow, VRootMeanSqr);
 fflush(fpvrms);
}



```

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 )
```

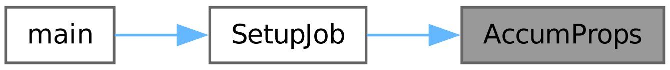
Definition at line 25 of file AccumProps.c.

```
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 ( )`

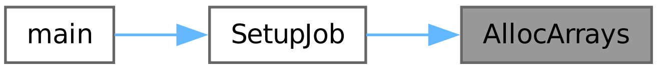
Definition at line 25 of file AllocArrays.c.

```
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.

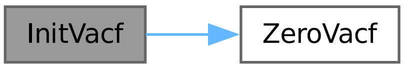
```
00026               {
00027   int nb;
00028   for(nb = 1 ; nb <= nBuffAcf ; nb ++)
00029     indexAcf[nb] = -(nb-1)*nValAcf/nBuffAcf;
```

```
  ZeroVacf();
}
```

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:

main
SetupJob
InitVacf

3.86.1.4 SetupJob()

```
void SetupJob ( )
```

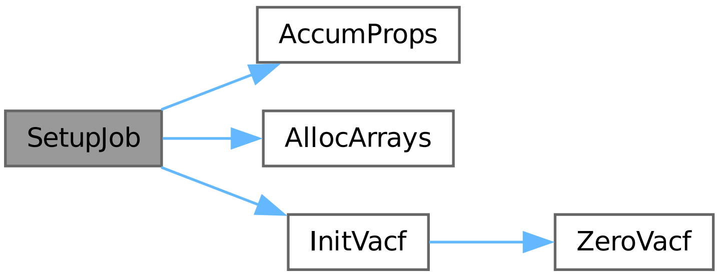
Definition at line 27 of file SetupJob.c.

```
                  {
  AllocArrays();
  AccumProps(0);
  InitVacf();
  stepCount = 0;
  // INITIALISE SPACETIME CORRELATIONS
  int n;
  for (n = 1; n <= nBuffCorr; n++)
    indexCorr[n] = -(n - 1)*nValCorr/nBuffCorr;

  countCorrAv = 0.;

  for (n = 1; n <= nFunCorr*nValCorr; n++)
    spacetimeCorrAv[n] = 0.;

  //RDF
  countRdf = 0;
}
```

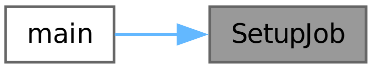
References AccumProps(), AllocArrays(), countCorrAv, countRdf, indexCorr, InitVacf(), nBuffCorr, nFunCorr, nValCorr, spacetimeCorrAv, and stepCount.

Referenced by main().

Here is the call graph for this function:



Here is the caller graph for this function:



3.87 SetupJob.c

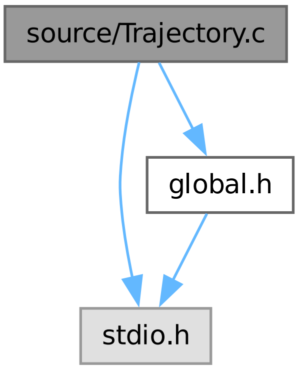
Go to the documentation of this file.

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

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

 */

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

void AllocArrays();
void AccumProps(int icode);
void InitVacf();
void SetupJob(){
  AllocArrays();
  AccumProps(0);
  InitVacf();
  stepCount = 0;
  // INITIALISE SPACETIME CORRELATIONS
  int n;
  for (n = 1; n <= nBuffCorr; n++)
    indexCorr[n] = -(n - 1)*nValCorr/nBuffCorr;

  countCorrAv = 0.;

  for (n = 1; n <= nFunCorr*nValCorr; n++)
    spacetimeCorrAv[n] = 0.;

  //RDF
  countRdf = 0;
}
```

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 ( )
```

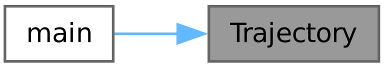
Definition at line 25 of file Trajectory.c.

```
                    {
  int n;
  //Trajectory file in LAMMPS dump format for OVITO visualization
  fprintf(fpxyz, "ITEM: TIMESTEP\n");
  fprintf(fpxyz, "%lf\n",timeNow);
  fprintf(fpxyz, "ITEM: NUMBER OF ATOMS\n");
  fprintf(fpxyz, "%d\n",nAtom);
  fprintf(fpxyz, "ITEM: BOX BOUNDS pp ff pp\n");
  fprintf(fpxyz, "%lf %lf xlo xhi\n", -regionH[1], regionH[1]);
  fprintf(fpxyz, "%lf %lf ylo yhi\n", -regionH[2], regionH[2]);
  fprintf(fpxyz, "%lf %lf zlo zhi\n", -0.1, 0.1);
  fprintf(fpxyz, "ITEM: ATOMS id mol type radius x y vx vy fx fy\n");
  for(n=1; n<=nAtom; n++)
   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",
  atomID[n], molID[n], atomType[n], atomRadius[n], rx[n], ry[n], vx[n], vy[n], ax[n], ay[n]);
}
```

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

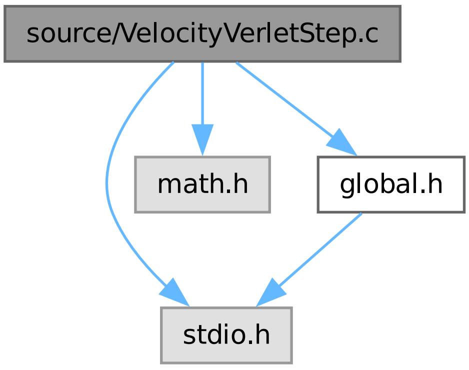
Go to the documentation of this file.

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

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

 */


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

void Trajectory(){
 int n;
 //Trajectory file in LAMMPS dump format for OVITO visualization
 fprintf(fpxyz, "ITEM: TIMESTEP\n");
 fprintf(fpxyz, "%lf\n",timeNow);
 fprintf(fpxyz, "ITEM: NUMBER OF ATOMS\n");
 fprintf(fpxyz, "%d\n",nAtom);
 fprintf(fpxyz, "ITEM: BOX BOUNDS pp ff pp\n");
 fprintf(fpxyz, "%lf %lf xlo xhi\n", -regionH[1], regionH[1]);
 fprintf(fpxyz, "%lf %lf ylo yhi\n", -regionH[2], regionH[2]);
 fprintf(fpxyz, "%lf %lf zlo zhi\n", -0.1, 0.1);
 fprintf(fpxyz, "ITEM: ATOMS id mol type radius x y vx vy fx fy\n");
 for(n=1; n<=nAtom; n++)
  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",
  atomID[n], molID[n], atomType[n], atomRadius[n], rx[n], ry[n], vx[n], vy[n], ax[n], ay[n]);
}



```

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

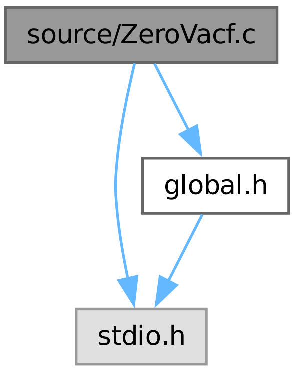
Go to the documentation of this file.

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

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

 */


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

void VelocityVerletStep(int icode){
int n;
 if(icode == 1){
 for (n= 1; n <= nAtom; n++) {
  if(atomType[n] != freezeAtomType){
  vx[n] += ax[n] * 0.5 * deltaT;
  vy[n] += ay[n] * 0.5 * deltaT;
  rx[n] += vx[n] * deltaT;
  ry[n] += vy[n] * deltaT;
  }
  //Calculating the image flags here
  if (rx[n] >= regionH[1]) {
   rx[n] -= region[1];
   ImageX[n]++;
   } else if (rx[n] < -regionH[1]) {
   rx[n] += region[1];
  ImageX[n]--;
  }
  if (ry[n] >= regionH[2]) {
   ry[n] -= region[2];
   ImageY[n]++;
   } else if (ry[n] < -regionH[2]) {
   ry[n] += region[2];
   ImageY[n]--;
   } } }
  else if(icode == 2){
  for(n = 1; n <= nAtom; n++) {
  if(atomType[n] != freezeAtomType){
   vx[n] += ax[n] * 0.5 * deltaT;
   vy[n] += ay[n] * 0.5 * deltaT;
} } } }

```

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

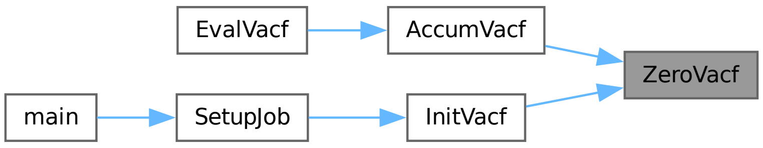
3.92.1.1 ZeroVacf()

```
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.

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

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

 */


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

void ZeroVacf(){
 int j;
 countAcfAv= 0 ;
 for(j = 1 ; j <= nValAcf ; j ++)
  viscAcfAv[j] = 0.;
}
```

Index