

Molecular Dynamics Code for Noble Gases  
1.0

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# Chapter 1

## File Index

### 1.1 File List

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<a href="#">headers.h</a>	Contains the function headers . . . . .	<a href="#">13</a>
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## Chapter 2

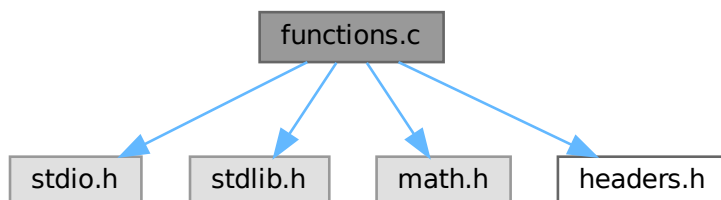
# File Documentation

### 2.1 functions.c File Reference

Contains the functions associated with the molecular dynamics simulation.

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

Include dependency graph for functions.c:



#### Functions

- double \*\* [allocate\\_2d\\_array](#) (int rows, int cols)  
*Allocates a 2D array of doubles.*
- void [free\\_2d\\_array](#) (double \*\*array, int rows)  
*Frees a 2D array from memory.*
- int [read\\_natoms](#) (const char \*filename)  
*Reads the number of atoms from an input file.*
- void [read\\_coords\\_and\\_masses](#) (const char \*filename, double \*\*coords, double \*masses, int n\_atoms)  
*Reads atomic coordinates and masses from an input file.*
- int [validate\\_atoms](#) (double \*masses, double \*epsilon, double \*sigma, int n\_atoms)  
*Validates that all atoms in the system are argon.*

- FILE \* [open\\_output](#) (const char \*filename)  
*Opens a file for writing output.*
- void [print\\_output](#) (FILE \*trajectory\_file, FILE \*energy\_file, FILE \*extended\_file, FILE \*acceleration\_file, int n\_atoms, int step, double kinetic\_energy, double potential\_energy, double total\_energy, double \*\*coords, double \*\*velocities, double \*\*accelerations)  
*Prints simulation output.*
- void [initialize\\_velocities](#) (double \*\*velocities, double \*masses, double temperature, int n\_atoms)  
*Initialize random velocities.*
- void [calculate\\_distances](#) (double \*\*coords, double \*\*distances, int n\_atoms)  
*Calculates distances between all pairs of atoms.*
- static double [lennard\\_jones\\_potential](#) (double r, double epsilon, double sigma)  
*Calculates the Lennard-Jones potential between two atoms.*
- double [calculate\\_potential\\_energy](#) (double \*\*distances, int n\_atoms, double epsilon, double sigma)  
*Calculates total potential energy of the system.*
- double [calculate\\_kinetic\\_energy](#) (double \*\*velocities, double \*masses, int n\_atoms)  
*Calculates total kinetic energy of the system.*
- double [calculate\\_total\\_energy](#) (double kinetic\_energy, double potential\_energy)  
*Calculates total energy of the system.*
- void [check\\_energy](#) (double previous\_energy, double total\_energy, int step)  
*Checks energy conservation between simulation steps.*
- void [thermostat](#) (double kinetic\_energy, double temperature, double \*\*velocities, int n\_atoms)  
*Velocity-rescaling thermostat.*
- static double [calculate\\_U](#) (double r, double epsilon, double sigma)  
*Helper function for acceleration calculation.*
- void [calculate\\_accelerations](#) (double \*\*coords, double \*masses, int n\_atoms, double epsilon, double sigma, double \*\*distances, double \*\*accelerations)  
*Calculates acceleration vectors for all atoms.*
- void [update\\_positions](#) (double \*\*coords, double \*\*velocities, double \*\*accelerations, double dt, int n\_atoms)  
*Updates atomic positions using Verlet algorithm.*
- void [update\\_velocities](#) (double \*\*velocities, double \*\*accelerations, double dt, int n\_atoms)  
*Updates atomic velocities using Verlet algorithm.*

## 2.1.1 Detailed Description

Contains the functions associated with the molecular dynamics simulation.

## 2.1.2 Function Documentation

### 2.1.2.1 [allocate\\_2d\\_array\(\)](#)

```
double ** allocate_2d_array (
    int rows,
    int cols )
```

Allocates a 2D array of doubles.

#### Parameters

<i>rows</i>	Number of rows in the array
<i>cols</i>	Number of columns in the array



### Returns

Pointer to the allocated 2D array

### Exceptions

<i>Exits</i>	with code 1 if memory allocation fails
--------------	----------------------------------------

#### 2.1.2.2 calculate\_accelerations()

```
void calculate_accelerations (
    double ** coords,
    double * masses,
    int n_atoms,
    double epsilon,
    double sigma,
    double ** distances,
    double ** accelerations )
```

Calculates acceleration vectors for all atoms.

#### Parameters

<i>coords</i>	Array of atomic coordinates
<i>masses</i>	Array of atomic masses
<i>n_atoms</i>	Number of atoms
<i>epsilon</i>	Epsilon parameter for LJ potential
<i>sigma</i>	Sigma parameter for LJ potential
<i>distances</i>	2D array of pairwise distances
<i>accelerations</i>	Array to store calculated accelerations

#### 2.1.2.3 calculate\_distances()

```
void calculate_distances (
    double ** coords,
    double ** distances,
    int n_atoms )
```

Calculates distances between all pairs of atoms.

#### Parameters

<i>coords</i>	Array of atomic coordinates
<i>distances</i>	2D array to store pairwise distances
<i>n_atoms</i>	Number of atoms

#### 2.1.2.4 calculate\_kinetic\_energy()

```
double calculate_kinetic_energy (
    double ** velocities,
    double * masses,
    int n_atoms )
```

Calculates total kinetic energy of the system.

##### Parameters

<i>velocities</i>	Array of atomic velocities
<i>masses</i>	Array of atomic masses
<i>n_atoms</i>	Number of atoms

##### Returns

Total kinetic energy of the system

#### 2.1.2.5 calculate\_potential\_energy()

```
double calculate_potential_energy (
    double ** distances,
    int n_atoms,
    double epsilon,
    double sigma )
```

Calculates total potential energy of the system.

##### Parameters

<i>distances</i>	2D array of pairwise distances
<i>n_atoms</i>	Number of atoms
<i>epsilon</i>	Epsilon parameter for LJ potential
<i>sigma</i>	Sigma parameter for LJ potential

##### Returns

Total potential energy of the system

#### 2.1.2.6 calculate\_total\_energy()

```
double calculate_total_energy (
    double kinetic_energy,
    double potential_energy )
```

Calculates total energy of the system.

## Parameters

<i>kinetic_energy</i>	Current kinetic energy
<i>potential_energy</i>	Current potential energy

## Returns

Total energy of the system

**2.1.2.7 calculate\_U()**

```
static double calculate_U (  
    double r,  
    double epsilon,  
    double sigma ) [static]
```

Helper function for acceleration calculation.

## Parameters

<i>r</i>	Distance between atoms
<i>epsilon</i>	Epsilon parameter for LJ potential
<i>sigma</i>	Sigma parameter for LJ potential

## Returns

U value

**2.1.2.8 check\_energy()**

```
void check_energy (  
    double previous_energy,  
    double total_energy,  
    int step )
```

Checks energy conservation between simulation steps.

## Parameters

<i>previous_energy</i>	Energy from previous step
<i>total_energy</i>	Current total energy
<i>step</i>	Current simulation step

## Warning

Prints warning if energy varies by more than 10%

### 2.1.2.9 free\_2d\_array()

```
void free_2d_array (
    double ** array,
    int rows )
```

Frees a 2D array from memory.

#### Parameters

<i>array</i>	Pointer to the 2D array to be freed
<i>rows</i>	Number of rows in the array

### 2.1.2.10 initialize\_velocities()

```
void initialize_velocities (
    double ** velocities,
    double * masses,
    double temperature,
    int n_atoms )
```

Initialize random velocities.

#### Parameters

<i>velocities</i>	Array of velocities
<i>masses</i>	Array of masses
<i>temperature</i>	Temperature
<i>n_atoms</i>	Number of atoms

### 2.1.2.11 lennard\_jones\_potential()

```
static double lennard_jones_potential (
    double r,
    double epsilon,
    double sigma ) [static]
```

Calculates the Lennard-Jones potential between two atoms.

#### Parameters

<i>r</i>	Distance between atoms
<i>epsilon</i>	Epsilon parameter for LJ potential
<i>sigma</i>	Sigma parameter for LJ potential

#### Returns

Value of the Lennard-Jones potential

### 2.1.2.12 open\_output()

```
FILE * open_output (
    const char * filename )
```

Opens a file for writing output.

#### Parameters

<i>filename</i>	Name of the output file
-----------------	-------------------------

#### Returns

Pointer to the opened file

#### Exceptions

<i>Exits</i>	with code 1 if file cannot be opened
--------------	--------------------------------------

### 2.1.2.13 print\_output()

```
void print_output (
    FILE * trajectory_file,
    FILE * energy_file,
    FILE * extended_file,
    FILE * acceleration_file,
    int n_atoms,
    int step,
    double kinetic_energy,
    double potential_energy,
    double total_energy,
    double ** coords,
    double ** velocities,
    double ** accelerations )
```

Prints simulation output.

#### Parameters

<i>trajectory_file</i>	File pointer for trajectory output
<i>energy_file</i>	File pointer for energy output
<i>extended_file</i>	File pointer for extended information
<i>acceleration_file</i>	File pointer for acceleration data
<i>n_atoms</i>	Number of atoms
<i>step</i>	Current simulation step
<i>kinetic_energy</i>	Current kinetic energy
<i>potential_energy</i>	Current potential energy
<i>total_energy</i>	Current total energy
<i>coords</i>	Array of atomic coordinates
<i>velocities</i>	Array of atomic velocities
<i>accelerations</i>	Array of atomic accelerations

### 2.1.2.14 read\_coords\_and\_masses()

```
void read_coords_and_masses (
    const char * filename,
    double ** coords,
    double * masses,
    int n_atoms )
```

Reads atomic coordinates and masses from an input file.

#### Parameters

<i>filename</i>	Name of the input file
<i>coords</i>	2D array to store coordinates
<i>masses</i>	Array to store atomic masses
<i>n_atoms</i>	Number of atoms

#### Exceptions

<i>Exits</i>	with code 1 if file cannot be opened
--------------	--------------------------------------

### 2.1.2.15 read\_natoms()

```
int read_natoms (
    const char * filename )
```

Reads the number of atoms from an input file.

#### Parameters

<i>filename</i>	Name of the input file
-----------------	------------------------

#### Returns

Number of atoms

#### Exceptions

<i>Exits</i>	with code 1 if file cannot be opened
--------------	--------------------------------------

### 2.1.2.16 thermostat()

```
void thermostat (
    double kinetic_energy,
    double temperature,
    double ** velocities,
    int n_atoms )
```

Velocity-rescaling thermostat.

**Parameters**

<i>kinetic_energy</i>	Kinetic energy
<i>temperature</i>	Desired temperature
<i>velocities</i>	Velocities
<i>n_atoms</i>	Number of atoms

**2.1.2.17 update\_positions()**

```
void update_positions (
    double ** coords,
    double ** velocities,
    double ** accelerations,
    double dt,
    int n_atoms )
```

Updates atomic positions using Verlet algorithm.

**Parameters**

<i>coords</i>	Array of atomic coordinates
<i>velocities</i>	Array of atomic velocities
<i>accelerations</i>	Array of atomic accelerations
<i>dt</i>	Time step
<i>n_atoms</i>	Number of atoms

**2.1.2.18 update\_velocities()**

```
void update_velocities (
    double ** velocities,
    double ** accelerations,
    double dt,
    int n_atoms )
```

Updates atomic velocities using Verlet algorithm.

**Parameters**

<i>velocities</i>	Array of atomic velocities
<i>accelerations</i>	Array of atomic accelerations
<i>dt</i>	Time step
<i>n_atoms</i>	Number of atoms

**2.1.2.19 validate\_atoms()**

```
int validate_atoms (
    double * masses,
```



```
double * epsilon,  
double * sigma,  
int n_atoms )
```

Validates that all atoms in the system are argon.

#### Parameters

<i>masses</i>	Array of atomic masses
<i>epsilon</i>	Pointer to store the epsilon parameter
<i>sigma</i>	Pointer to store the sigma parameter
<i>n_atoms</i>	Number of atoms

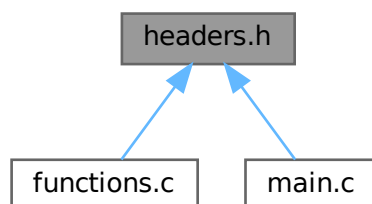
#### Returns

1 if all atoms are valid, 0 otherwise

## 2.2 headers.h File Reference

Contains the function headers.

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



#### Macros

- #define [CONSTANTS\\_H](#)
- #define [ARGON\\_MASS](#) 39.948
- #define [ARGON\\_EPSILON](#) 0.0661
- #define [ARGON\\_SIGMA](#) 0.3345
- #define [PI](#) 3.14159265358979323846
- #define [R](#) 8.31446261815324

## Functions

- double \*\* [allocate\\_2d\\_array](#) (int rows, int cols)  
*Allocates a 2D array of doubles.*
- void [free\\_2d\\_array](#) (double \*\*array, int rows)  
*Frees a 2D array from memory.*
- int [read\\_natoms](#) (const char \*filename)  
*Reads the number of atoms from an input file.*
- void [read\\_coords\\_and\\_masses](#) (const char \*filename, double \*\*coords, double \*masses, int n\_atoms)  
*Reads atomic coordinates and masses from an input file.*
- int [validate\\_atoms](#) (double \*masses, double \*epsilon, double \*sigma, int n\_atoms)  
*Validates that all atoms in the system are argon.*
- void [initialize\\_velocities](#) (double \*\*velocities, double \*masses, double temperature, int n\_atoms)  
*Initialize random velocities.*
- void [calculate\\_distances](#) (double \*\*coords, double \*\*distances, int n\_atoms)  
*Calculates distances between all pairs of atoms.*
- double [calculate\\_potential\\_energy](#) (double \*\*distances, int n\_atoms, double epsilon, double sigma)  
*Calculates total potential energy of the system.*
- double [calculate\\_kinetic\\_energy](#) (double \*\*velocities, double \*masses, int n\_atoms)  
*Calculates total kinetic energy of the system.*
- double [calculate\\_total\\_energy](#) (double kinetic\_energy, double potential\_energy)  
*Calculates total energy of the system.*
- void [thermostat](#) (double kinetic\_energy, double temperature, double \*\*velocities, int n\_atoms)  
*Velocity-rescaling thermostat.*
- void [check\\_energy](#) (double previous\_energy, double total\_energy, int step)  
*Checks energy conservation between simulation steps.*
- void [calculate\\_accelerations](#) (double \*\*coords, double \*masses, int n\_atoms, double epsilon, double sigma, double \*\*distances, double \*\*accelerations)  
*Calculates acceleration vectors for all atoms.*
- void [update\\_positions](#) (double \*\*coords, double \*\*velocities, double \*\*accelerations, double dt, int n\_atoms)  
*Updates atomic positions using Verlet algorithm.*
- void [update\\_velocities](#) (double \*\*velocities, double \*\*accelerations, double dt, int n\_atoms)  
*Updates atomic velocities using Verlet algorithm.*
- FILE \* [open\\_output](#) (const char \*filename)  
*Opens a file for writing output.*
- void [print\\_output](#) (FILE \*trajectory\_file, FILE \*energy\_file, FILE \*extended\_file, FILE \*acceleration\_file, int n\_atoms, int step, double kinetic\_energy, double potential\_energy, double total\_energy, double \*\*coords, double \*\*velocities, double \*\*accelerations)  
*Prints simulation output.*

## 2.2.1 Detailed Description

Contains the function headers.

## 2.2.2 Macro Definition Documentation

### 2.2.2.1 ARGON\_EPSILON

```
#define ARGON_EPSILON 0.0661
```

### 2.2.2.2 ARGON\_MASS

```
#define ARGON_MASS 39.948
```

### 2.2.2.3 ARGON\_SIGMA

```
#define ARGON_SIGMA 0.3345
```

### 2.2.2.4 CONSTANTS\_H

```
#define CONSTANTS_H
```

### 2.2.2.5 PI

```
#define PI 3.14159265358979323846
```

### 2.2.2.6 R

```
#define R 8.31446261815324
```

## 2.2.3 Function Documentation

### 2.2.3.1 allocate\_2d\_array()

```
double ** allocate_2d_array (
    int rows,
    int cols )
```

Allocates a 2D array of doubles.

#### Parameters

<i>rows</i>	Number of rows in the array
<i>cols</i>	Number of columns in the array

#### Returns

Pointer to the allocated 2D array

#### Exceptions

<i>Exits</i>	with code 1 if memory allocation fails
--------------	----------------------------------------

### 2.2.3.2 calculate\_accelerations()

```
void calculate_accelerations (
    double ** coords,
    double * masses,
    int n_atoms,
    double epsilon,
    double sigma,
    double ** distances,
    double ** accelerations )
```

Calculates acceleration vectors for all atoms.

#### Parameters

<i>coords</i>	Array of atomic coordinates
<i>masses</i>	Array of atomic masses
<i>n_atoms</i>	Number of atoms
<i>epsilon</i>	Epsilon parameter for LJ potential
<i>sigma</i>	Sigma parameter for LJ potential
<i>distances</i>	2D array of pairwise distances
<i>accelerations</i>	Array to store calculated accelerations

### 2.2.3.3 calculate\_distances()

```
void calculate_distances (
    double ** coords,
    double ** distances,
    int n_atoms )
```

Calculates distances between all pairs of atoms.

#### Parameters

<i>coords</i>	Array of atomic coordinates
<i>distances</i>	2D array to store pairwise distances
<i>n_atoms</i>	Number of atoms

### 2.2.3.4 calculate\_kinetic\_energy()

```
double calculate_kinetic_energy (
    double ** velocities,
    double * masses,
    int n_atoms )
```

Calculates total kinetic energy of the system.

#### Parameters

<i>velocities</i>	Array of atomic velocities
<i>masses</i>	Array of atomic masses
<i>n_atoms</i>	Number of atoms

**Returns**

Total kinetic energy of the system

**2.2.3.5 calculate\_potential\_energy()**

```
double calculate_potential_energy (
    double ** distances,
    int n_atoms,
    double epsilon,
    double sigma )
```

Calculates total potential energy of the system.

**Parameters**

<i>distances</i>	2D array of pairwise distances
<i>n_atoms</i>	Number of atoms
<i>epsilon</i>	Epsilon parameter for LJ potential
<i>sigma</i>	Sigma parameter for LJ potential

**Returns**

Total potential energy of the system

**2.2.3.6 calculate\_total\_energy()**

```
double calculate_total_energy (
    double kinetic_energy,
    double potential_energy )
```

Calculates total energy of the system.

**Parameters**

<i>kinetic_energy</i>	Current kinetic energy
<i>potential_energy</i>	Current potential energy

**Returns**

Total energy of the system

**2.2.3.7 check\_energy()**

```
void check_energy (
    double previous_energy,
    double total_energy,
    int step )
```

Checks energy conservation between simulation steps.

**Parameters**

<i>previous_energy</i>	Energy from previous step
<i>total_energy</i>	Current total energy
<i>step</i>	Current simulation step

**Warning**

Prints warning if energy varies by more than 10%

**2.2.3.8 free\_2d\_array()**

```
void free_2d_array (
    double ** array,
    int rows )
```

Frees a 2D array from memory.

**Parameters**

<i>array</i>	Pointer to the 2D array to be freed
<i>rows</i>	Number of rows in the array

**2.2.3.9 initialize\_velocities()**

```
void initialize_velocities (
    double ** velocities,
    double * masses,
    double temperature,
    int n_atoms )
```

Initialize random velocities.

**Parameters**

<i>velocities</i>	Array of velocities
<i>masses</i>	Array of masses
<i>temperature</i>	Temperature
<i>n_atoms</i>	Number of atoms

**2.2.3.10 open\_output()**

```
FILE * open_output (
    const char * filename )
```

Opens a file for writing output.

## Parameters

<i>filename</i>	Name of the output file
-----------------	-------------------------

## Returns

Pointer to the opened file

## Exceptions

<i>Exits</i>	with code 1 if file cannot be opened
--------------	--------------------------------------

## 2.2.3.11 print\_output()

```
void print_output (
    FILE * trajectory_file,
    FILE * energy_file,
    FILE * extended_file,
    FILE * acceleration_file,
    int n_atoms,
    int step,
    double kinetic_energy,
    double potential_energy,
    double total_energy,
    double ** coords,
    double ** velocities,
    double ** accelerations )
```

Prints simulation output.

## Parameters

<i>trajectory_file</i>	File pointer for trajectory output
<i>energy_file</i>	File pointer for energy output
<i>extended_file</i>	File pointer for extended information
<i>acceleration_file</i>	File pointer for acceleration data
<i>n_atoms</i>	Number of atoms
<i>step</i>	Current simulation step
<i>kinetic_energy</i>	Current kinetic energy
<i>potential_energy</i>	Current potential energy
<i>total_energy</i>	Current total energy
<i>coords</i>	Array of atomic coordinates
<i>velocities</i>	Array of atomic velocities
<i>accelerations</i>	Array of atomic accelerations

## 2.2.3.12 read\_coords\_and\_masses()

```
void read_coords_and_masses (
    const char * filename,
```

```
double ** coords,
double * masses,
int n_atoms )
```

Reads atomic coordinates and masses from an input file.

#### Parameters

<i>filename</i>	Name of the input file
<i>coords</i>	2D array to store coordinates
<i>masses</i>	Array to store atomic masses
<i>n_atoms</i>	Number of atoms

#### Exceptions

<i>Exits</i>	with code 1 if file cannot be opened
--------------	--------------------------------------

### 2.2.3.13 read\_natoms()

```
int read_natoms (
    const char * filename )
```

Reads the number of atoms from an input file.

#### Parameters

<i>filename</i>	Name of the input file
-----------------	------------------------

#### Returns

Number of atoms

#### Exceptions

<i>Exits</i>	with code 1 if file cannot be opened
--------------	--------------------------------------

### 2.2.3.14 thermostat()

```
void thermostat (
    double kinetic_energy,
    double temperature,
    double ** velocities,
    int n_atoms )
```

Velocity-rescaling thermostat.



## Parameters

<i>kinetic_energy</i>	Kinetic energy
<i>temperature</i>	Desired temperature
<i>velocities</i>	Velocities
<i>n_atoms</i>	Number of atoms

**2.2.3.15 update\_positions()**

```
void update_positions (
    double ** coords,
    double ** velocities,
    double ** accelerations,
    double dt,
    int n_atoms )
```

Updates atomic positions using Verlet algorithm.

## Parameters

<i>coords</i>	Array of atomic coordinates
<i>velocities</i>	Array of atomic velocities
<i>accelerations</i>	Array of atomic accelerations
<i>dt</i>	Time step
<i>n_atoms</i>	Number of atoms

**2.2.3.16 update\_velocities()**

```
void update_velocities (
    double ** velocities,
    double ** accelerations,
    double dt,
    int n_atoms )
```

Updates atomic velocities using Verlet algorithm.

## Parameters

<i>velocities</i>	Array of atomic velocities
<i>accelerations</i>	Array of atomic accelerations
<i>dt</i>	Time step
<i>n_atoms</i>	Number of atoms

**2.2.3.17 validate\_atoms()**

```
int validate_atoms (
    double * masses,
```

```
double * epsilon,
double * sigma,
int n_atoms )
```

Validates that all atoms in the system are argon.

#### Parameters

<i>masses</i>	Array of atomic masses
<i>epsilon</i>	Pointer to store the epsilon parameter
<i>sigma</i>	Pointer to store the sigma parameter
<i>n_atoms</i>	Number of atoms

#### Returns

1 if all atoms are valid, 0 otherwise

## 2.3 headers.h

[Go to the documentation of this file.](#)

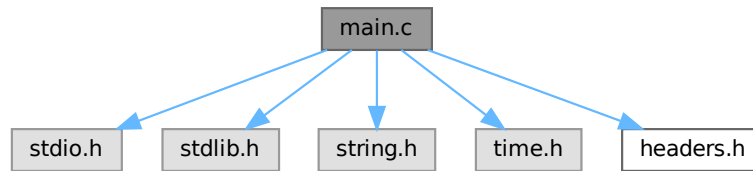
```
00001
00006 #ifndef FUNCTIONS_H
00007 #define FUNCTIONS_H
00008
00009 double** allocate_2d_array(int rows, int cols);
00010 void free_2d_array(double** array, int rows);
00011 int read_natoms(const char* filename);
00012 void read_coords_and_masses(const char* filename, double** coords, double* masses, int n_atoms);
00013 int validate_atoms(double* masses, double* epsilon, double* sigma, int n_atoms);
00014 void initialize_velocities(double** velocities, double* masses, double temperature, int n_atoms);
00015 void calculate_distances(double** coords, double** distances, int n_atoms);
00016 double calculate_potential_energy(double** distances, int n_atoms, double epsilon, double sigma);
00017 double calculate_kinetic_energy(double** velocities, double* masses, int n_atoms);
00018 double calculate_total_energy(double kinetic_energy, double potential_energy);
00019 void thermostat(double kinetic_energy, double temperature, double** velocities, int n_atoms);
00020 void check_energy(double previous_energy, double total_energy, int step);
00021 void calculate_accelerations(double** coords, double* masses, int n_atoms, double epsilon, double
sigma, double** distances, double** accelerations);
00022 void update_positions(double** coords, double** velocities, double** accelerations, double dt, int
n_atoms);
00023 void update_velocities(double** velocities, double** accelerations, double dt, int n_atoms);
00024 FILE* open_output(const char* filename);
00025 void print_output(FILE* trajectory_file, FILE* energy_file, FILE* extended_file, FILE*
acceleration_file, int n_atoms, int step, double kinetic_energy, double potential_energy, double
total_energy, double** coords, double** velocities, double** accelerations);
00026 #endif
00027
00028 // Constants
00029 #ifndef CONSTANTS_H
00030 #define CONSTANTS_H
00031
00032 #define ARGON_MASS 39.948
00033 #define ARGON_EPSILON 0.0661 // j/mol
00034 #define ARGON_SIGMA 0.3345 // nm
00035 #define PI 3.14159265358979323846
00036 #define R 8.31446261815324 // Ideal gas constant in J/K/mol
00037
00038 #endif
```

## 2.4 main.c File Reference

Contains the main program.

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

```
#include <string.h>
#include <time.h>
#include "headers.h"
Include dependency graph for main.c:
```



## Functions

- `int main (int argc, char *argv[ ])`  
*The main entry point of the program.*

### 2.4.1 Detailed Description

Contains the main program.

### 2.4.2 Function Documentation

#### 2.4.2.1 main()

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

The main entry point of the program.

This program manages reading of the input, performing the MD simulation and generation of output.

#### Returns

int Returns 0 upon successful execution.

### 2.4.3 Variables

- `int n_steps`: Number of simulation steps.
  - `double dt`: Time step.
  - `double temperature`: Temperature.
  - `int thermo`: If set to 1, the thermostat is activated, if set to 0 it is deactivated.
  - `const char* filename`: Name of the input file.
  - `int n_atoms`: Number of atoms.
  - `double** coords`: 2D array of coordinates consisting of x, y, z for each atom.
  - `double** distances`: 2D array of distances for each pair of atoms.
  - `double* masses`: Array of masses of each atom.
  - `double epsilon`: Epsilon parameter for the Lennard-Jones potential in j/mol.
  - `double sigma`: Sigma parameter for the Lennard-Jones potential in nm.
  - `double** velocities`: 2D array of velocities consisting of vx, vy, vz for each atom.
  - `double** accelerations`: 2D array of accelerations consisting of ax, ay, az for each atom.
  - `const char* trajectory_name`: Name of the file where the trajectory output is written.
  - `FILE* trajectory_file`: File where the trajectory output is written.
  - `const char* energy_name`: Name of the file where the energies are written.
  - `FILE* energy_file`: File where the energies are written.
  - `const char* extended_name`: Name of the file where the extended trajectory with velocities is written.
  - `FILE* extended_file`: File where the extended trajectory with velocities is written.
  - `const char* acceleration_name`: Name of the file where the accelerations are written.
  - `FILE* acceleration_file`: File where the accelerations are written.
  - `double kinetic_energy`: Variable for storing the kinetic energy.
  - `double potential_energy`: Variable for storing the potential energy.
  - `double total_energy`: Variable for storing the total energy.
  - `double previous_energy`: Variable for storing the total energy of the previous step.
- Name of the input file

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