MD

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Here are the classes, structs, unions and interfaces with brief descriptions:

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File Index

2.1 File List

Here is a list of all documented files with brief descriptions:

Chapter 3

Class Documentation

3.1 constants Module Reference

Public Member Functions

- subroutine inital (x, v, a)

    generate inital position and velocity
- subroutine cal_f (x, f, E_V)

    calculate force and potential energy of particles
- subroutine cal_et (v, E_T)

    calculate kinetic energy
- subroutine cal_v (f0, f, a, v0, v, E_T)

    calculate velocity of particles

Public Attributes

- real(8), parameter temperture =275.0

    Temperture Temperture, unit of K !
- real(8), parameter dt =1.0E-16

    Time interval, unit of s !
- real(8), parameter tmax =1.0E-12

    Max simulation time, unit of s.
- real(8), parameter l =1.0E-9

    Cell length, unit of m.
- real(8), parameter rc =6.85E-10

    Cut off, unit of m.
- real(8), parameter kb =1.38E-23

    Boltzmann constant, unit of J/K.
- real(8), parameter m =3.35E-26

    Mass of Ne, unit of kg.
- real(8), parameter sigma =2.74E-10

    Lennard-Jones-sigma.
- real(8), parameter e =5.0E-22

    Lennard-Jones-e.
- real(8), parameter freq =0.01

    Andersen thermostat collision frequence.
- integer, parameter npart =100

> *Number of particle.*

- integer, parameter nsample =10

    Sampling step lengths.

- real(8), parameter rc2 =rc∗∗2

    Sqrt of Cut off, unit of m.

- real(8), parameter pi =3.141592657

    constant pi

3.1.1   Detailed Description

Definition at line 29 of file MD.f90.

The documentation for this module was generated from the following file:

- MD.f90

Chapter 4

File Documentation

4.1 MD.f90 File Reference

FUNCTIONS: MD.

Data Types

- module constants

Functions/Subroutines

- program main

    program main

4.1.1 Detailed Description

FUNCTIONS: MD.

A simple NVT MD simulation program. Use Lennard-Jones Potential, Velocity Verlet Algorithm, Andersen Thermostat.

Author

Wenqiang Li

Parameters

Temperture	Temperture, unit of K
dt	Time interval, unit of s
tmax	Max simulation time, unit of s
L	Cell length, unit of m
rc	Cut off, unit of m
kb	Boltzmann constant, unit of J/K
m	Mass of Ne, unit of kg
sigma	Lennard-Jones-sigma

e	Lennard-Jones-e
freq	Andersen thermostat collision frequence
npart	Number of particle
nsample	Sampling step lengths
rc2=rc∗∗2	Sqrt of Cut off, unit of m