A Simple Implementation of MD for Lennard Jones Fluid

1. Simulation Details

a. Simulation parameters

Use the parameters are in reduced units, with the choice for the basic units as, we can have the simulation parameters as the following,

T^*	ρ^*	V^*	m^*	r^*
0.728	0.8442	V/ε	m/m_{atom}	r/σ

The simulation box size is thus determined with the density

$$\frac{108}{L^3} = 0.8442$$

b. Initialization

The initial location of the atoms are assigned using the simple cubic lattice structure.

And the velocities are randomly drawn from the Gaussian distribution. To achieve zero net momentum, the velocities in each direction is subtracted by the mean value. To set the initial temperature, the initial velocities are scaled using the following relationship,

$$\frac{3}{2}Nk_BT = \frac{1}{2}\sum_i mv_i^2$$

c. Force calculation

The LJ-potential is simplified as,

$$V(r) = 4\left[\frac{1}{r^{12}} - \frac{1}{r^6}\right]$$

with $r_{ij} = r_i - r_j$, the force applied to i^{th} atom due to i^{th} atom is,

$$\boldsymbol{F_{ij}} = -\frac{\partial V}{\partial r} = \left(\frac{48}{r_{ij}^{14}} - \frac{24}{r_{ij}^{8}}\right)\boldsymbol{r_{ij}}$$

and the force exerted on i^{th} atom is thus,

$$\boldsymbol{F_i} = \sum_j \boldsymbol{F_{ij}}$$

Using truncated and shifted potential,

$$\mathrm{V}_{\mathrm{trun,sh}}^{LJ}(r) = \begin{cases} V^{LJ}(r) - V^{LJ}(r_c) & when\ r \le r_c \\ 0 & when\ r > r_c \end{cases}$$

the pair force becomes,

$$\boldsymbol{F}_{ij} = -\frac{\partial V}{\partial r_{ij}} = \begin{cases} \left(48\frac{1}{r_{ij}^{14}} - 24\frac{1}{r_{ij}^{8}}\right)\boldsymbol{r_{ij}}, & when\ r \le r_c \\ 0, & when\ r > r_c \end{cases}$$

The force applied to j^{th} atom due to the i^{th} atom is thus given by,

$$F_{ji} = -F_{ij}$$

d. Periodic Boundary Condition

Minimum image convention is adopted for the force calculation in periodic boundary condition. When the atoms exits the domain, it re-enter the domain from the opposite boundary.

e. Time Forward Algorithm

Time integration using velocity verlet algorithm, its corresponding implementation:

1st half step:

$$v\left(t + \frac{1}{2}\Delta t\right) = v(t) + \frac{1}{2}\frac{F_i(t)}{m_i}\Delta t$$

$$r_i(t + \Delta t) = r_i(t) + v\left(t + \frac{1}{2}\Delta t\right)\Delta t$$

2nd half step,

$$v_i(t+\Delta t) = v\left(t+\frac{1}{2}\Delta t\right)\Delta t + \frac{1}{2}\frac{F_i(t+\Delta t)}{m_i}\Delta t$$

f. Sampling of the energy

The kinetic energy, potential energy and total energy is calculated by taking average of the corresponding values after the equilibrating the system.

g. Radial Distribution Function (RDF)

The number of atoms $N(r+\frac{1}{2}\Delta r)$ in each bin $(r, r+\Delta r)$ for each atom at each time frame is counted, then the average is taken,

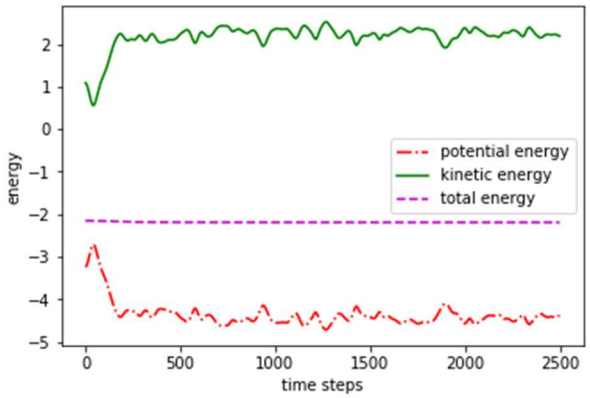
$$n\left(r+\frac{1}{2}\Delta r\right) = \frac{N\left(r+\frac{1}{2}\Delta r\right)}{N_t \cdot N_{atom}}$$

The RDF $g(r)$ is then normalized with the density and volume in the bin as,

$$g\left(r+\frac{1}{2}\Delta r\right) = \frac{n\left(r+\frac{1}{2}\Delta r\right)}{\frac{4}{3}\pi((r+\Delta r)^3 - r^3)\cdot\rho}$$

2. Results

(1). The evolution plot for the kinetic energy, potential energy and total energy per particle.

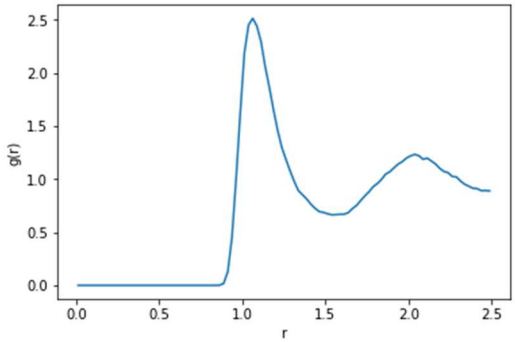


(2). The potential energy, kinetic energy and total energy per particle after equilibration.

Quantity	K/N	U/N	(K+U)/N
My MD	2.245050	-4.437931	-2.192881
Reference	2.2564±0.0012	-4.4190±0.0012	-2.1626±0.0024

The results are quite close but still slightly differently from the reference values.

(3). The radial distribution function $g(r)$.



3. Appendix – source code

The code is in python as listed in the following pages.