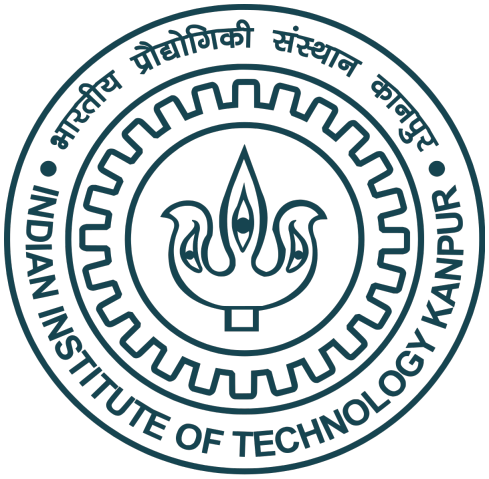
Project Report - CHM684A

Molecular Dynamics Simulation of liquid Argon

Group Members:
Chitresh Bhaskar Chaudhari
Sharad Dattatray Gaikwad
Saarthak Shrivastava

Indian Institute of Technology, Kanpur



Contents

Problem Statement

In this project, the Molecular Dynamics (MD) Simulation of liquid Argon (Ar) has been performed and then the Radial Distribution Function, Mean Square Displacement has been calculated from the simulation trajectory and compared with results in the reference article[1].

1 Introduction And Motivation

The calculations presented here are based on the assumption that classical dynamics with a two-body central-force interaction can give a reasonable description of the motion of atoms in liquid argon. For practical reasons, further assumptions have to be made, namely, the interaction potential has to be truncated beyond a certain range, the number of particles in the assembly has to be kept rather small, and suitable boundary conditions have to be imposed on the assembly. Finally, the equations of motion have to be solved as a set of difference equations, thus involving a certain increment of time to go from one set of positions and velocities to the next.

1.1 Lennard Jones Potential

The Lenard Jones potential is given by:-

$$U(R_1, R_2, R_3, ..., R_n) = 4\epsilon \sum_{I<J} [(\frac{\sigma}{R_{ij}})^{12} - (\frac{\sigma}{R_{ij}})^{6}]$$

$$R_{ij} = |Ri - Rj|$$

ϵ=Depth of potential
σ=Distance before which the repulsive term in the potential contributes

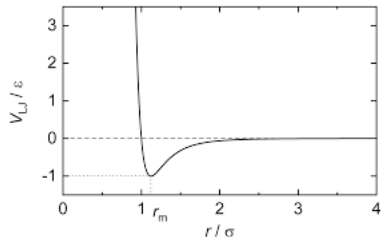


Figure 1: Lennard-Jones potential

[1] A. Rahman (1964) Correlations in the Motion of Atoms in Liquid Argon, Phys. Rev. 136, A405.

1.2 Box-Muller Sampling

Maxwell distribution of velocities at temperature T :-

$$f(v) = [(\frac{M}{2\pi k_b T})^{1/2} \exp(\frac{-Mv^2}{2k_b T})]$$

$$X = \sigma \cos(2\pi\xi_1)\sqrt{-2\ln\xi_2'}$$

$$Y = \sigma \sin(2\pi\xi_1)\sqrt{-2\ln\xi_2'}$$

$$\sigma = \sqrt{\frac{k_b T}{M}}$$

X & Y are two random velocities picking randomly from the f(v) at temperature T

1.3 Mean-Square Displacement

$$< r^2 >= \frac{1}{N}\frac{1}{n_{t_0}} \sum_{t_0} \sum_{i}^{N} (\mathbf{r}_i(t_0 - t) - \mathbf{r}_i(t_0))^2$$

Here, is N the number of particles, t is the time and t_0 is the time origin. Also, n_{t_0} is the number of time origins considered for averaging.

1.4 Velocity-Verlet Integrator

Velocity-Verlet Integrator has been used to integrate the equations of motion. The general algorithm for Velocity-Verlet Integrator is as follows:

$$v(t + \Delta t/2) = v(t) + \frac{\Delta t}{2} a(t)$$

$$r(t + \Delta t/2) = r(t) + \Delta t v(t + \Delta t/2)$$

$$v(t + \Delta t) = v(t + \Delta t/2) + \frac{\Delta t}{2} a(t + \Delta t)$$

2 Method and Model

2.1 Model

We used 4 modules and main project file for this project as follows:

- PROGRAM main
- MODULE variables
- MODULE md
- MODULE gr

- MODULE rmsdisplacement

Module variables contains all necessary variables required in program. Module md contains all the subroutines required to do molecular dynamics of argon gas. Module gr contains subroutine to calculate radial distribution function. module rmsdisplacement contains subroutine to calculate $< r^2 >$.

2.2 Method

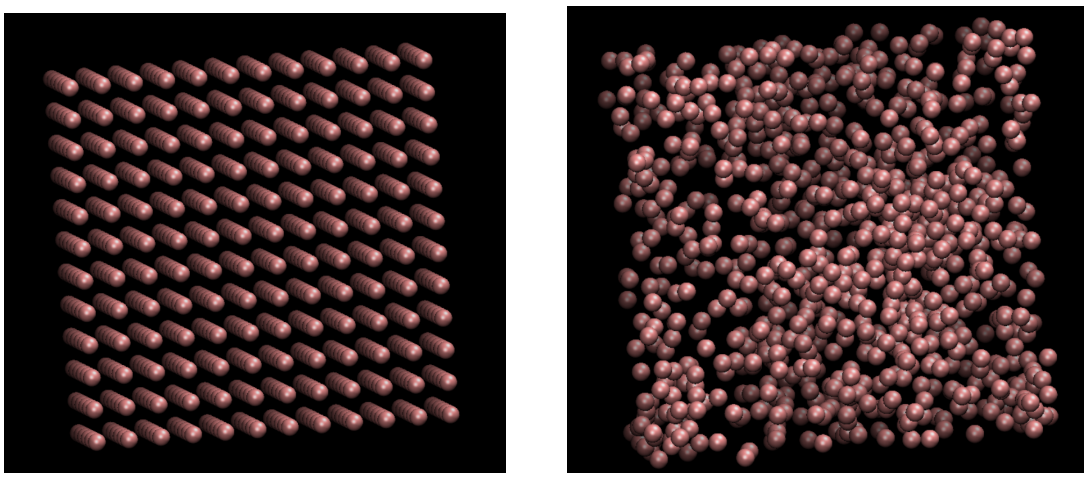
- First the main program main.f90 calls SUBROUTINE create_lattice(). This subroutine asks for number of atoms, density, temperature, step size and number of steps.
- After this, program call subroutine get_initial_velocities() to assign initial velocities to each atom. This velocities are assigned from the Maxwell-Boltzmann equation using the Box-Muller Sampling.
- After this function calls SUBROUTINE energy_forces() to calculate initial energy and forces.
- After this there is do loop iterating from 1 to maximum number of steps given by user. In this loop Velocity-Verlet Integrator has been used to integrate the equations of motion. There are individual subroutines to calculate using velocity-Verlet integrator.
- In the same loop, temperature is calculated for each step. Also after every 50 iteration program call subroutine to print coordinates of atoms and energies in different files.
- After the loop, program calls SUBROUTINE calculate_gr() which calculates radial distribution function and prints required information to plot g(r) vs r in separate file.
- At last, program call SUBROUTINE rmsd() which calculates root mean square displacement according to equation mentioned before.

2.3 Simulation details

- **Number of atoms** : 864
- **Density** : 1.374 g/cm^3 (0.8 in reduced unit)
- **Temperature** : 94.4 K (0.786 in reduced unit)
- **Time step** : 0.001 ps
- **Number of steps** : 10000

3 Results

3.1 Lattice structure



(a) snapshot of lattice before simulation

(b) Snapshot of lattice at the end of simulation

Figure 2: Lattice structure at start and end of the simulation

3.2 Energy vs Time

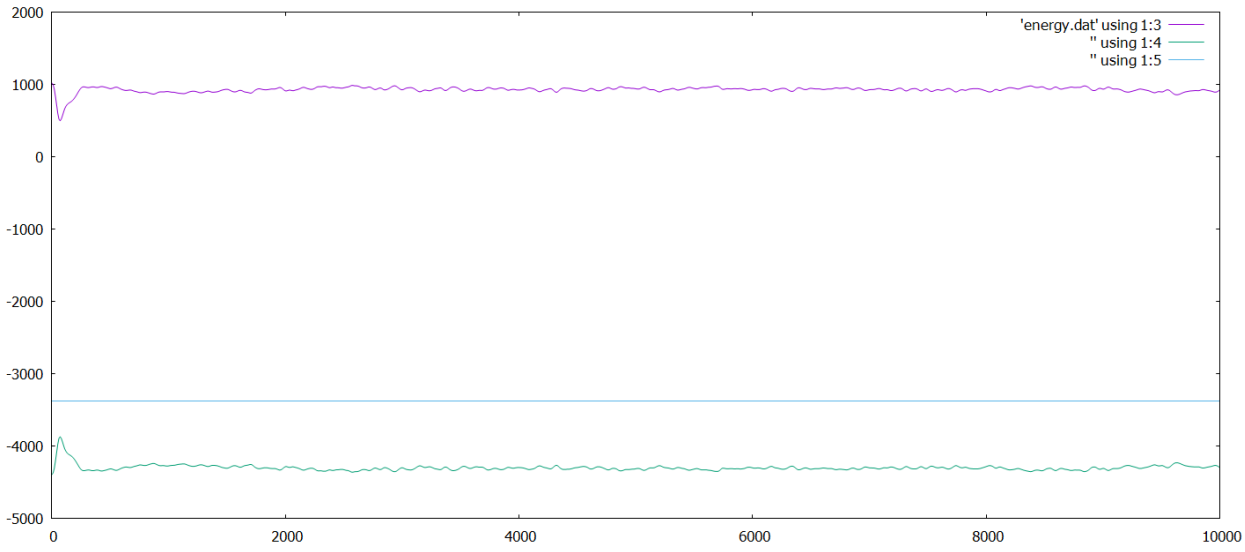


Figure 3: Energy as a function of number of steps

Fig 3 represents potential(green), kinetic(pink) and total(blue) energy as a function of number of steps. Here we can observe that there is no drift in the total energy. Potential and kinetic energy varies with time but total energy remains same throughout the simulation.

Temperature variance is as shown in fig 4: Temperature initially drop down but then

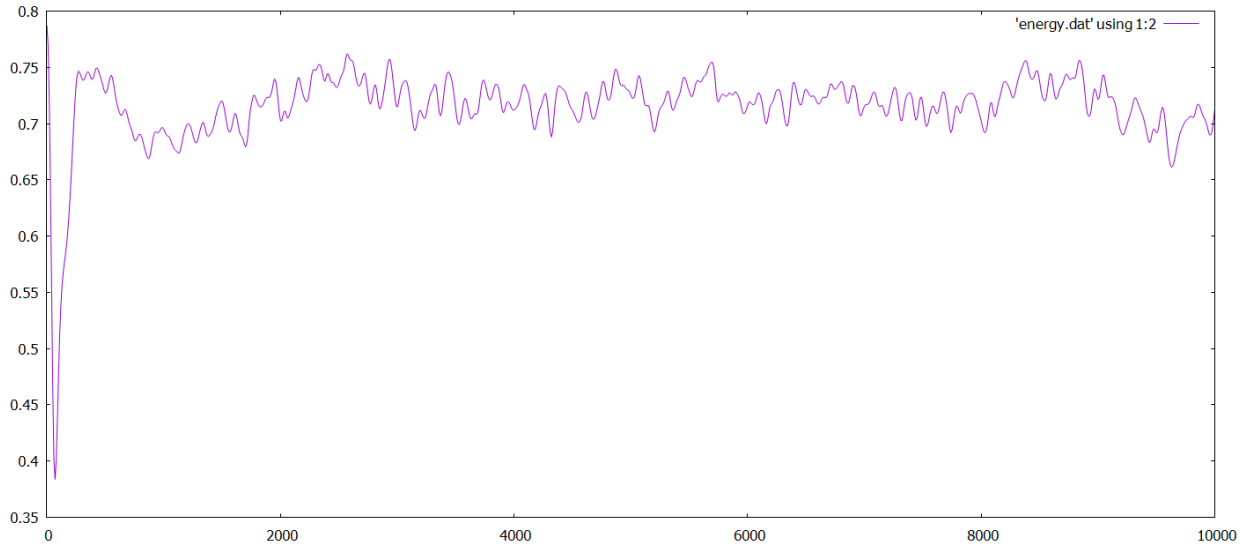


Figure 4: Temperature vs time in MD simulation

oscillate in near the simulation temperature through the simulation.

3.3 Radial Distribution function g(r)

Radial distribution is given the fig 5. Here we can see that, there is peak at 1σ and two smaller peaks near 2σ and 3σ.1 unit on x axis is equal to 3.7 $\mathring{A}$. The obtained plot exactly replicates the fig 2 of reference article.

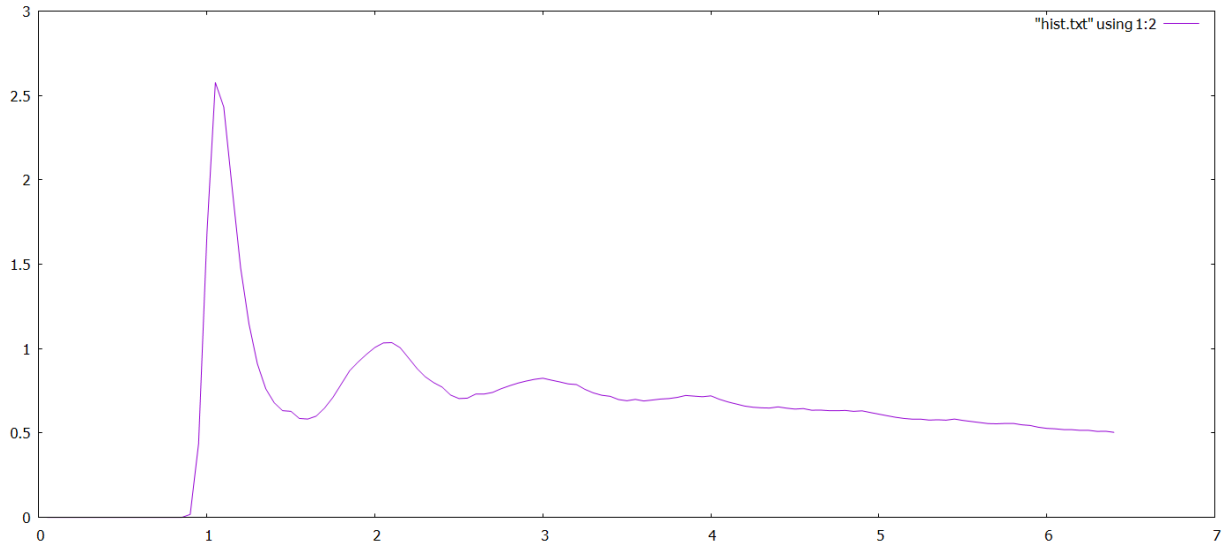


Figure 5: Radial Distribution Function g(r)

3.4 Mean Square Displacement $< r^2 >$

Fig 6 shows root mean square displacement as a function of time. It is very similar to fig 3 of reference article.

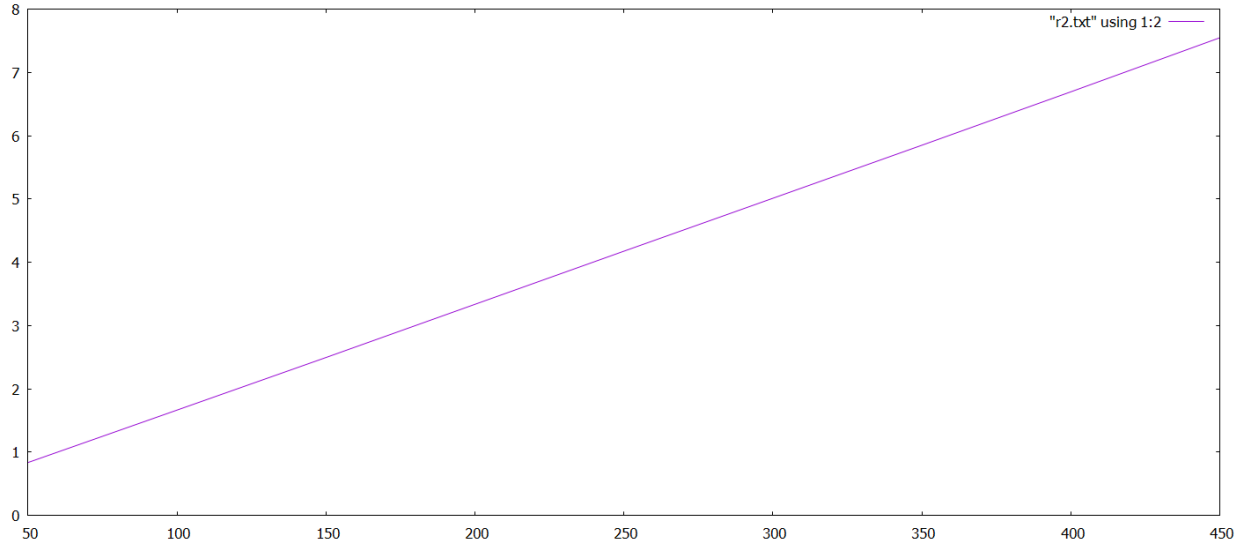


Figure 6: Root mean square displacement - $< r^2 >$

4 Conclusion

We tried to replicate results of paper by A. Rahman in this project. We succeeded in showing absence of drift in total energy. Also, we managed plot radial distribution function and root mean squarte displacement plots identical to the plots in refererece article. In summary, we successfully replicated the experiment done by A. Rahman.

Acknowledgement

We would like to thank Prof. Nisanth Nair and Mr. Saurabh Srivastav for Motivating and guiding us throughout the project.