12 NOVEMBER 2020

CHM684A

# PROJECT-2B

**SET2 B**

**NOV 12, 2020**

# MOLECULAR DYNAMICS SIMULATION OF LIQUID ARGON

In this project, you will be reproducing the landmark paper by A. Rahman (A. Rahman, Phys. Rev. 136, A405; https://journals.aps.org/pr/abstract/10.1103/PhysRev.136.A405), which is considered to be the first report of molecular dynamics simulation of a realistic system.

In this work, he has used a system of three dimensional 864 Lennard-Jones particles to simulate liquid Argon.

The potential energy of interaction will be based on the Lennard-Jones function discussed in my lectures (Lecture 21A). Use the parameters of the simulation (such as Temperature, Density, system size, $\sigma$, $\epsilon$ etc.) as the same as that in the aforementioned paper. You can use the velocity scaling to maintain the instantaneous temperature if It deviates beyond the window 94.4±10 K. Apply Periodic Boundary Conditions. Use the

velocity Verlet integrator for integrating the equations. Initial velocities are to be assigned from the Maxwell-Boltzmann equation using the Box-Muller Sampling.

1. Show that your implementation is working by showing that there is no drift in total energy when 1 fs time step is used.

2. Generate the radial-distribution function, $g(r)$, and compare with Figure 2 of the paper. (See Project 1B fore more on the algorithm for computing $g(r)$)

3. Compute mean-square displacement of particles:

$$\left\langle r^2 \right\rangle = \frac{1}{N}\frac{1}{n_{t_0}} \sum_{t_0} \sum_{i}^{N} \left( \mathbf{r}_i(t_0 + t) - \mathbf{r}_i(t_0) \right)^2$$

Here, $N$ is 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. You may choose the time points separated by 1000 frames as time origins. Make a plot of $\left\langle r^2 \right\rangle$ as a function of time and compare with Figure 3 of the paper.

# IMPLEMENTATION

You need to write Fortran modular programs,: (i) For doing MD , (ii) for the computation of $g(r)$, and (iii) for the computation of mean-square-displacement $\left\langle r^2 \right\rangle$.

The program (i) should contain subroutines for
a) Constructing initial structure (lattice) and initial velocities (Box-Muller)
a) Velocitiy Verlet Integrator
b) Periodic boundary condition
c) Computing energy and forces
d) Computing instantaneous temperature, kinetic energy, potential energy and total energy
e) Write energies to the output.
c) Write XYZ file for every 50 steps (in the same file, in appended mode)
d) Wrapping coordinates within the box before writing the XYZ file

Use pointers for storing coordinates, forces, and velocities. The MD program should read in number of atoms, density, temperature, time step, and number of steps. The input keywords should be read-in as "in-line commands". The $g(r)$ and the mean-square-displacement codes should to read-in the .xyz trajectory file. Both these codes should read number of atoms and number of frames in the .xyz files directly from the .xyz file. Other input parameters should be read-in by "in-line commands".

# REPORT

The report should contain introduction to the problem and aim of the project. Subsequently, "Methods and Models" part should give details about the model, algorithm, program design, and other technical/theoretical details. The details given here should help someone else to reproduce your results. In the "Results" part, explain the results with figures (and tables if needed). All the tables and figures should have captions, with figure/table numbers. Generate the figures of the last snapshot of the trajectory (by visualising .xyz through VMD) , energy plots (Total Energy, Potential Energy, Kinetic Energy), $g(r)$ and $\langle r^2 \rangle$. Indicate the units in the axis while making plots. Final section of the report should be "Conclusion" where you conclude the results of your work. You can add the codes to the report as Appendix.