

Master's in Computational Modelling in Physics, Chemistry and Biochemistry
COURSE: MOLECULAR MODELLING
DEPARTMENT: FÍSICA DE LA MATÈRIA CONDENSADA
ACADEMIC YEAR: 2022-2023

1. Write / Adapt a simple Molecular Dynamics Simulations code.

Write down a Molecular Dynamics Simulations code for a system of N particles interacting through a Lennard-Jones potential in contact with a heat bath.

- (a) Describe in detail the different parts of the code. How do you initialize the system of particles (and set the density)? What integrator do you use? How do you implement periodic boundary conditions? How do you control the temperature (how do you implement the thermostat)? What units do you use for the Lennard-Jones interactions? What cut-off do you use for the interactions (and why)? What truncation strategy do you choose?
- (b) Perform a simulation of an isolated system (no contact with thermal bath) of $N > 100$ Lennard-Jones particles:
 - i. Initialize the positions so that the system has a density $\rho = 0.7m/\sigma^3$. Initialize the velocities with a bimodal distribution for each component so that its kinetic energy is compatible with a temperature $k_B T = 100\epsilon$, where σ and ϵ are the typical parameters of the Lennard-Jones potential.
 - ii. Run your simulation using a velocity Verlet integrator and check that the total energy and the total momentum of the system are conserved as time advances. Test your results for different values of the timestep and describe your results. Show the plots of the energy and momentum as a function of time and discuss the results.
 - iii. Do the same tests (also with different values of the timestep) using the Euler integrator and describe your results.
 - iv. Calculate and show the velocity distribution of the particles in the beginning of the simulation and after the system has equilibrated. Calculate the temperature of the system after equilibration. Show that the distribution of velocities after equilibration obtained from your simulation follows a Maxwell-Boltzmann distribution.

2. Analysis of properties of a Lennard-Jones liquid. Considering that the interaction between argon atoms can be described using a Lennard-Jones potential with $\epsilon = 0.998\text{kJ/mol}$ and $\sigma = 3.4\text{\AA}$ (and the atomic mass of argon is $m = 40\text{g/mol}$):

- (a) Calculate the kinetic, potential and total energy per particle of a system of ($N > 100$) argon atoms in a fluid state with densities $\rho = 0.05, 0.1, 0.2, 0.4, 0.6, 0.8m/\sigma^3$ and a fixed temperature (using a thermal bath) $k_B T = 1.2\epsilon$.
 - Plot a graph with the kinetic, potential and total energy as a function of density. Show your results in units of kJ/mol for the energies and g/cm³ for the density. How do you equilibrate your system? How many timesteps do you use to calculate your results?
 - Visualize (part of) the equilibrium trajectory and interpret your observations in terms of the phase diagram of the Lennard-Jones fluid shown in Fig. 1.
- (b) Calculate the pressure of a system of ($N > 100$) argon atoms at $k_B T = 1.2\epsilon$ for densities $\rho = 0.05, 0.1, 0.2, 0.4, 0.6, 0.8m/\sigma^3$. Plot your results in Pascal.
- (c) (extra 1) Calculate the mean square displacement over time of argon atoms in a system of $N > 100$ particles with $\rho_1 = 0.05m/\sigma^3$ and $\rho_1 = 0.8m/\sigma^3$ at $k_B T = 1.2\epsilon$. Extract the corresponding diffusion coefficient of argon atoms. Show the plot of the mean square displacement (in units of \AA^2) versus time (in units of picoseconds). Interpret your results in terms of the phase diagram of the Lennard-Jones fluid shown in Fig. 1.
- (d) (extra 2) Obtain the radial distribution function of argon at $k_B T = 2.0\epsilon$ and $\rho = 0.8m/\sigma^3$. Show the plot of the radial distribution function versus distance in units of \AA .

In an appendix to the final report, list the simulation and analysis codes that you have written.

Hint: To produce the thermodynamic results use as many timesteps as possible ($N_{steps} > 100000$).

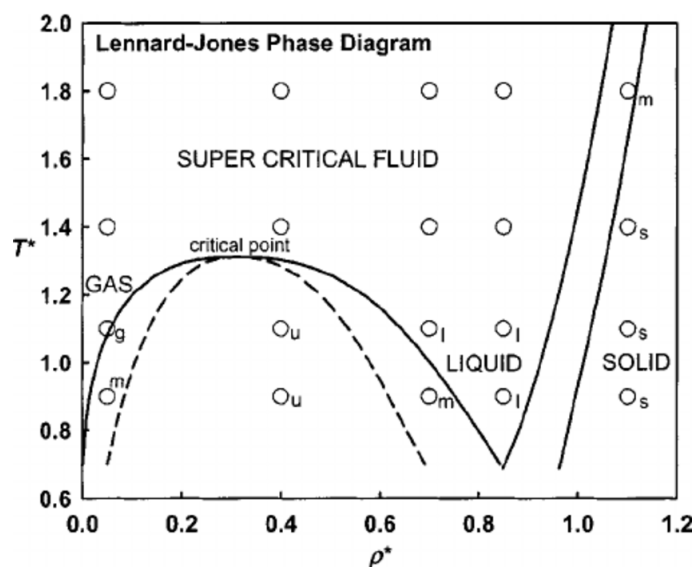


FIG. 1: Phase diagram of Lennard-Jones fluid in reduced units