Problem Set 7: Chemistry 175/273

This homework is due on Gradescope by class time on Mar. 12, 2025.

1. *Lennard-Jones simulation*

   Using the template provided, you will conduct some small scale numerical experiments to model noble gas dynamics.

   (a) Plot the Lennard-Jones potential for $\epsilon = 1, 2, 5$ and describe your expectation for the effect of ϵ on the state of the system at fixed temperature.

   (b) Compute the interatomic force as a function of interparticle distance r for a pair of particles.

   (c) Using the template provided, modify the initialization function so that you can specify the initial temperature (in units of k_{B}).

   (d) We have provided a function that computes interparticle distance (here we use periodic boundary conditions, meaning that if you exit the box on the right, you return on the left, etc.). Implement a function that computes the total potential energy of the system.

   (e) Implement a function that returns the force vector between each pair of particles i and j. Note that your output will be a tensor with shape $n \times n \times 2$.

   (f) Implement a function that simultaneously computes the force and the energy (it will have the same content as above, but you can combine the loops to save some computational time).

   (g) Initializing simulations at $T = 1, 2$, and 5, compute the average kinetic energy of the system over a trajectory of 5000 time steps.

   (h) *Extra credit:* At $T = 1$, compute the radial distribution function $g(r)$ for a density in the gas phase and a density in liquid phase. A good estimate will require simulations longer than those used in the previous problem.

   (i) *Even more extra credit:* Compute the first virial coefficient $B(T)$ numerically for $T = 1, 2, 3, 4, 5$ in the liquid phase.