Physics 5403: Computational Physics – Project 7a

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due date: Nov 15, 2022

Molecular dynamics simulation of a Lennard-Jones gas

In this project you will perform a classical molecular dynamics simulation for a gas of particles interacting via the Lennard-Jones potential

$$V_{LJ}(r_{ij}) = -4\epsilon \left[(\sigma/r_{ij})^6 - (\sigma/r_{ij})^{12} \right]$$

where r_{ij} is the distance between atoms i and j. For argon, the parameters are $\epsilon = 0.0104$ eV and $\sigma = 3.40$Å, and the atomic mass is 39.95 amu. The typical particle density at room temperature and ambient pressure is $0.0269/\mathrm{nm}^3$ whereas the particle density of the liquid at the boiling point (87.3 K) is $21.0/\mathrm{nm}^3$. The goal of this project is to determine the equation of state, i.e the relation between temperature, pressure, and volume, the specific heat and the pair distribution function.

1. Write a program which integrates Newton's equations of motion of N particles in a cubic box of linear size L (periodic boundary conditions) from $t_{min} = 0$ to t_{max} with time step τ. It may be convenient to measure all length in units of σ and all energies and temperature in units of ϵ.

   Your external parameters are particle number, volume and total energy. Think about how to initialize positions and velocities.

2. Start with a small system of about 50 particles. Measure kinetic and potential energies after each step. Use the requirement of energy conservation to find a reasonable time step τ starting from a guess based on the parameter values given above.

3. Plot a few trajectories and inspect them to get an idea concerning the equilibration time. You will want to see a number of collisions between particles during your simulation window. Substantiate your guess for the equilibration time by following the kinetic and potential energies separately. What behavior do you expect? What do you observe?

4. Implement the calculation of observables, viz., temperature, pressure, and the pair distribution function. The temperature can be calculated from the kinetic energy using the equipartition theorem, the pressure from the virial theorem and the pair distribution directly from the positions.

5. Perform production runs in the temperature range from 0 to room temperature (how do you translate this into a range for the initial energy?) and a range of typical distances from about σ to 10σ. (Why is this the interesting range?)

6. Plot the pressure-temperature-volume relation (e.g. in a pressure-temperature diagram). How does it compare with the van der Waals equation

   $$(p + aN^2/V^2)(V - Nb) = Nk_BT?$$

7. Plot the energy-temperature relation and determine the specific heat.