Physics 5403: Computational Physics – Project 7b

due date: November 15, 2022

Simulated annealing of argon clusters

The goal of this project is to use simulated annealing to find the lowest energy structures of argon clusters. The total energy is given by $E = \frac{1}{2}\sum_{i\neq j} V(r_{ij})$ where r_{ij} is the distance between atoms i and j. The pair interaction between two ions at distance r can be modeled by a Lennard-Jones potential

$$V(r) = -4\epsilon\left[\left(\frac{\sigma}{r}\right)^6 - \left(\frac{\sigma}{r}\right)^{12}\right] .$$

The parameters for argon are: $\epsilon = 0.0104$ eV and $\sigma = 3.40$Å, and the atomic mass is 39.95 amu.

a) Write a molecular dynamics program that integrates Newton's equations of motion of N particles in a cubic box of linear size L from $t_{min} = 0$ to t_{max} with time step τ. It may be convenient to measure all lengths in units of σ and all energies and temperatures in units of ϵ.

   Add a temperature control loop that systematically reduces the temperature (kinetic energy) during the annealing procedure. Keep track of the lowest state reached during the run.

b) Test your program for clusters of 3 and 4 argon atoms. Think about how to choose the size of a confining box (if any) as well as the initial positions and velocities. Test how the rate of decrease of the temperature influences the results.

c) Consider larger clusters (for all integer N_p up to 13) and determine the energies and structure of the lowest energy configuration for each particle number.

d) Use the methods of project 5 to find the metastable states by direct minimization of the energy. Compare the lowest energies found by simulated annealing with those of the direct minimization. What can you do to further improve the results? Try to modify the temperature vs. time protocol!