PHYS580 Lab 12, November 14, 2019

Assignment: today's required lab activity is for a molecular dynamics simulation of a two-dimensional system of particles interacting via the so-called Lennard-Jones potential (cf. Chapter 9 in the textbook). On the course web page under Labs, you can find three relevant starter programs in Matlab: *md2.m* (main code), *updatemd.m* (performs one timestep), and *calc_energy.m* (calculates the current value of the energy).

1. Use the starter programs (or your own equivalent ones) to simulate a system of, say, 25 particles in a square of side length 5 (in units of σ, the Lennard-Jones parameter). Initially, let the particles be at rest but with a relatively small random variation in position from the evenly spaced, square lattice vertices. (Why give the variation?) Then, as the simulation proceeds, produce images of the time evolution of particle positions similar to those displayed in Fig. 9.6 of the textbook. Also reproduce the time series of the total energy, temperature, tagged particle and tagged pair separations. Are the fluctuations in energy and temperature, and the trend of the pair separation as you expect, and why?

2. How can you speed up the convergence to equilibrium you observed in (1)? Find out a way to do so using the feature of the starter program that allows one to change the kinetic energy of the particles via keyboard input during the simulation. Similarly, when you have attained a stable triangular arrangement of the particles (*solid*), find a way to *melt* it by heating it. Demonstrate that you succeeded in melting the crystal by making appropriate plots of the particle arrangements and the time series of various functions.

   Note: What happens if the time step is too large (small) or if you raise the temperature too much, and why? Address these in your discussion.

3. Study the effect of varying the density, initial velocities and/or positions on the approach to equilibrium and the nature of the final equilibrium configuration. You do not need to be exhaustive on this. For example, try putting 25 particles in a square of side length 10, and see how their characteristics change as you vary the temperature, substantiating your discussion using various time series graphs.