

Physics 325 — Scientific Computing — Fall 2016 — Lab 12

December 2, 2016

All exercises this week use the Monte Carlo program for the Argon atom Lennard-Jones potential in the notebook LJMD to be found on Piazza. Use it with modifications to to the following-

Exercise 1. Baseline calculations

Look over the LMJD program to get an idea of how it works. Then using at least 64 atoms and 400 steps, run the program and make plots of the initial particle distribution, final particle distribution, and a histogram plot of velocity squared for all particles. Comment on whether or not with some imagination the distribution of velocity squareds is looking like a Maxwell-Boltzmann distribution (look up a plot). **(10 points, 5 points extra credit for color coding the symbols for the final particle positions plot according to velocity).**

Exercise 2. Energetics

Modify the code, or add ancillary code to process the resulting data, to plot the total kinetic energy, potential energy, and total energy for the system of particles for each step. Comment on matters of conservation of energy. **(10 points)**

Extra Credit: Go Faster

The code as written spends twice as much time as necessary calculating the acceleration of the particles. This is because it loops over each particle, and then loops over all other particles calculating the net acceleration on a particle due to all others. In reality, Newton's 3rd law applies and the force of one particle on the other will just be equal and opposite to the force of the 2nd back on the first.

See if you can modify those loops (and it may require more careful definitions of the current and/or new variables) so that each force pair calculation is used twice instead of once, halving the number of times through the loops. **(10 points)**