Chemical Engineering I5800 Molecular Simulation Spring 2019

Problem Set 2 – due Feb. 28

1. Copy the programs mc_nvt.f, params.inc and fort.10 from the web site; this is a fortran program for Monte Carlo simulations of a Lennard-Jones system in the NVT ensemble, and a sample input data file. Read the program, and compile and run it with the original data file – this will run in seconds, and produce lots of explanatory output. Be sure that you understand *everything* in the program. If anything is not clear, ask me.

2. Write a (short) fortran program subroutine which reads the final positions from the output file fort.21 and produces a histogram of the one-dimensional density profile of the atoms, in the x-direction, say. Choose the bin width in the histogram so that most of them are occupied. The recast your program as a subroutine which is inserted into the main program mc_nvt.f so you can produce the *average* density profile. In this case you should call the subroutine periodically, store the results, and average them at the end. You can experiment with how often the subroutine is called: if it's too often the positions haven't changed much and the code is inefficient, but if it's called too infrequently the average will not be smooth. Likewise, you can experiment with the bin width: over time the entire x-axis is sampled so finer binning is appropriate. Note that you can let the system equilibrate once and for all if you do it once and then save and read the output from a file in subsequent runs.

3. As written, the program initializes the particle positions on a cubic lattice which uniformly fills a cube. Modify the program so that the initial positions are squeezed in the x-direction so that the atoms occupy only one third of the box; this requires changes in subroutine lattice. Run the program until the density becomes as uniform as it was before the modification. Compute *instantaneous* density profile at various times during the run to see how long it takes to stabilize. This can be done quantitatively if you invent a numerical criterion for when the density profile is flat enough. Compare the behavior of the density profiles to the variation of the energy and pressure with the number of steps; Does everything stabilize at the same time?

Hand in the code for the initial program and an indication of how the subroutine version is inserted into the main program, along with the final and average profiles in parts 2 and 3, and a discussion of the stabilization. Please hand in the numerical results for the evolution of the energy and the density profile with the number of MC steps, along with your density subroutine and any other modifications you made in the code. Please do *not* hand in the all of the screen output produced when the program runs.