Chemical Engineering I5800 Molecular Simulation Spring 2019

Problem Set 3 – due Mar. 14

1. Using the program mc_nvt.f, determine the pair distribution function $g(r)$ for three cases: temperature 1.0 and densities 0.2 and 0.8, and temperature 0.2 and density 0.8. The runs require simple changes in fort.10, and in each case you should compute g as an average over the production part of the run. Please submit the new code you've written and an indication of where it is inserted, and a plot of the result.

2. Simulate 100 Lennard-Jones atoms at temperature 1.0 and density 0.8 in the NVT ensemble, grouped into 50 diatomic rigid molecules of bond length σ, and find the energy and pressure. Look at subroutine lattice to decide how to pair up the atoms, and then use a mixture of translational and rotational Metropolis moves. Submit the modifications made to the code along with the results for pressure and energy.

3. Same as (1) but use soft molecular bonds based on a harmonic potential $\frac{1}{2}\,k(\mathbf{r}_1 - \mathbf{r}_2)^2$ with spring constant $k = 30 \cdot \epsilon/\sigma^2$. Also, compute the probability distribution of bond lengths, and compare the mean value to the position of the minimum of the net two-body potential (Lennard-Jones plus spring). Again, submit the modifications made in the code along with the the numerical results.

4. Using program mc_nvt.f with 100 atoms and temperature 1.0 and density 0.8, calculate the mean and the statistical error in the pressure and energy in equilibrium, using either the block average or the jackknife methods discussed in class.