PROBLEM SET 8

1. (a) Sketch (quantitatively) the radial distribution function for gaseous argon at T = 300 K, P = 1 bar.

(b) Calculate (analytically) the radial position, r_{max}, that corresponds to the maximum value of the radial distribution function for low-pressure argon. Is r_{max} a function of temperature?

Argon approximately follows the Lennard-Jones 12-6 potential with

$\varepsilon/k_B = 120$ K, $\sigma = 0.34$ nm

2. Consider a system consisting of a colloidal particle of radius σ and charge Q=+20e (e is the charge of an electron) stationary in the center of a spherical cavity of radius R=5σ. Its counterions have negligible size and can be at any distance between σ and R. Estimate the counterion distribution function, g(r), as a function of distance using a numerical solution of the Poisson-Boltzmann equations as described in the notes. In particular, perform the calculations at conditions so that the Bjerrum length $\xi = e^2/(4\pi\varepsilon\varepsilon_0 k_B T)$ is (a) $\xi = \sigma/5$ (b) the Bjerrum length is $\xi=\sigma/50$ and (c) $\xi=\sigma/2$. Also obtain the total energy of the system for these three cases. Note that is easier to work in reduced units, with length measured in units of σ and energy in units of $e^2/4\pi\varepsilon\varepsilon_0\sigma$.

3. Perform a Monte Carlo simulation of the system of part 2 and compare the results for the mean energy to the theoretical predictions of part 2. You may use any programming environment (e.g. C, Visual Basic, MATLAB, Fortran, Java …) available on the OIT cluster machines to which you have access. The code would set up the counterions in an initial random configuration and then perform displacement moves to sample configuration space, accepting or rejecting each one according to the Metropolis rules. You may want to output the total system energy periodically in order to analyze the results “off line.”