Assignment 4 – Due Dec. 1st by electronic submission to azp@princeton.edu

Problem 1

For this problem, you will need to use the GCMC code of assignment 2 – your own code, Frenkel+Smit's, or the one provided with my solution. Modify the code to obtain data for the frequency of observing a given energy and number of particles at (μ_0, T_0); then write a separate program (or use Matlab) to "reweight" the data to any desired combination of (μ, T). Illustrate how this approach works by obtaining data at $(\mu_0, T_0) = (-3.5, 1.3)$ for $L = 7$ and then using them to predict as much of the ρ-μ isotherm at $T = 1.4$ as possible. Compare the histogram reweighting predictions to a few actual runs at this new temperature.

Problem 2

[Exercise 14 from book] You are asked to use both Widom test particle insertions and the Gibbs ensemble to locate the vapor-liquid equilibrium point for the Lennard-Jones fluid.

(a) Modify the Monte Carlo code for the Lennard-Jones fluid in the *NVT* ensemble provided in the book web site (only in the file *mc_nvt.f*) to obtain the chemical potential using Widom insertions. You may also modify your own code (from assignment 2), but then you will need to add code to obtain the pressure as well as the energy. Locate the liquid and vapor coexistence densities at T=0.8.

(b) Use a Gibbs ensemble simulation to obtain the liquid and vapor coexistence densities at T=0.8. How do the results to compare?

Please submit your solution (graphs, comments, any code lines that you added) as a single PDF file similar to that provided as solution to assignment 1. I will assign 20% of the grade to "aesthetics" of your solution: how easy it is to follow, quality and proper labeling of graphs etc.