Physics G6080 – Problem Set 4
Due Friday March 29, 2013

1. The Monte Carlo method can be used to simulate argon liquid, at a given temperature, through the canonical ensemble. The results of a canonical simulation should agree very closely with the results of a microcanonical simulation (molecular dynamics), differing only due to the fact that the number of particles, while large, is not infinite.

   Your molecular dynamics code can be easily modified to do a Monte Carlo simulation by replacing the Verlet algorithm part of the code with a Metropolis update for each particle and velocity. Of course, you do not need to do the velocity via Monte Carlo, since it is a Maxwell distribution, but it is a negligible computational overhead to include it and it keeps the changes in your code small.

   Modify your argon molecular dynamics code to do a Monte Carlo simulation at a temperature of $T = 1.069$ and density $\rho = 0.75$. Measure the same variables as in problem set 3 and check that your answers agree. Include statistical errors for your results.

   In the molecular dynamics simulations, the autocorrelation times for observables are related to physical quantities, since the evolution represents real dynamics of the system. For the Monte Carlo, the autocorrelation times reflect the algorithm used for the update. Quote measured integrated autocorrelation times for the measured temperature.