

Problem Set 4 – due Mar. 21

1. Download and familiarize yourself with the programs for NpT Monte Carlo simulations from the course web site (mc_npt.f, npt_params.inc and fort.15). Run the program using the parameter set in fort.15 and determine the average volume. Then, using the volume you obtain from this calculation, run the previous NVT code at the same particle number, density and temperature and determine the pressure. It should agree with the pressure assumed in the NpT simulation.
2. Use the Widom particle insertion method to find the chemical potential for 100 particles at temperature 1.0 and density $0.3\sigma^{-3}$ using the NVT code. Be sure to test the stability of the results by examining the average value for different numbers of steps, and estimate the statistical uncertainty using the block variance method.