

Assignment 2 – Due Oct. 20, 2009, by electronic submission to azp@princeton.edu

The Lennard-Jones potential between two particles i and j at a distance r is:

$$U_{ij}(r) = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right]$$

1. Use NVT Monte Carlo to compute the isotherms at $T^*=1$ and 1.5 between densities of $\rho^*=0$ and $\rho^*=0.7$ for systems with $L^*=7$. Report the energy, statistical uncertainty (95% confidence interval) and CPU time required for each of your runs. How does the CPU time per MC step scale as a function of system size?
2. Use μVT Monte Carlo for the same system at the two temperatures and range of densities given above. Compare the results for the energy to those obtained with the NVT code. Report the energy, density, their statistical uncertainties (95% confidence interval) and CPU time required for each of your runs.

You may use Frenkel and Smit's codes as starting points, or write your own code from scratch. If you write your own code, make sure to submit a listing of it along with your results and comments, in a single .pdf file similar to that provided as solution to assignment 1.