
Homework Assignment #4 - Due March 11

Monte Carlo Simulations - Hard Sphere and Ising Model

In this exercise, you will perform Monte Carlo simulations of Hard Sphere systems and 2D Ising Models.

Please use our **class nanoHUB tool** with the Hard Sphere and Ising codes for this work.

Hard Sphere Monte Carlo

- Recall that you will need to adjust the Metropolis displacement D to achieve an acceptance rate around 50%. You need not be too strict on this. In fact, so long as the acceptance rate fluctuates between 0.4 and 0.6, you are fine. Be careful -- the acceptance rate can change in the course of the run.

- As an input temperature, choose T=2.0 in our energy unit which is simply the height of the potential core, and choose the density to be 1.0 particles per cubic sigma. Choose the number of particles to be initially 36, in 3 dimensions.

- Calculate the energy per particle, as well as the pressure, which is not automatically produced as output by the code. You should use the expression below for the pressure, but taking into account the discontinuity of the potential. (You can look for help, for example, in the book by Gould and Tobochnick, page 594).

$$\frac{P}{kT} = \rho - \frac{\rho^2}{6kT}\int r\frac{dv}{dr}g(r)4\pi r^2 dr$$

- Look at the 10 plots of the pair distribution function: what can you conclude about the state of the system?
- Lower the temperature to T=1 and T=0.1; do you see anything happening by looking at the pair distribution functions?
- Now repeat this study with 128 particles at the same density, qualitatively and/or quantitatively. Does the displacement required to achieve 50% acceptance change?
- Repeat the above calculation at a density 0.5. Do you see the same things you saw at the previous density?

Ferromagnetic-Paramagnetic Transition in the 2D Ising Model

- Estimate the transition temperature for the ferro-para magnetic transition for the 2D Ising Model as well as the magnetic susceptibility of the system.
- Choose two of the following system sizes: 4x4, 8x8, or 16x16.
- For each of these, vary the temperature from 1.3 to 3.4 in increments of 0.3.
- Hint: be sure that you use sufficiently long runs for each simulation. You need to generate enough data to accurately compute averages and errors. This will require runs of around 5000 Monte Carlo steps.
- Using the results on the magnetization of the system, estimate the transition temperature and the susceptibility.
- How does the size of the system affect your results?
- To get a complete data set, you can send your results to Elif by Thursday March 6th. I will compile everyone's data together and make it available here so you can see the final results. Your final task then is to explain what you see, estimate the transition temperature, and estimate the susceptibility.
