Thermal Physics: Monte Carlo Projects

The final assignment for this course will be to compute the equilibrium properties of some non-trivial interacting system using Monte Carlo simulation techniques. Here I suggest four doable projects which I hope you will find to be interesting. Of course if you have something else in mind, please see me. I would like you to work in teams of two and each team must do a different project. The following project descriptions are not overly detailed since part of this assignment is to do some background work on your topic. I can suggest some references in each case. During the final week of classes each group will give a 20 minute presentation on their project and results. You will be required to turn in a written summary of your MC algorithm and of your results along with a working version of your simulation code. I'd prefer you to work in Matlab which will allow you to easily generate some graphical output to go along with your project. I'd like everyone to start thinking about these projects now and tell me what you'll be doing by next week. Remember, I want to see different projects and it's first come first serve, so the sooner you tell me, the better chance you have of getting your pick.

Project #1 (Ryogo & Richard): Ising Model Phase Transition: Finite size scaling and critical exponents

Second order phase transitions, such as that exhibited by the 2D Ising model, are generally characterized by a power law behavior of thermodynamic variables near the transition. One typically observes the form $|(1-T/T_c)|^{-p}$ where T_c is the critical temperature and p is known as the critical exponent. Systems displaying the same critical exponents are said to belong to the same universality class. For the Ising model (in zero magnetic field), the specific heat, magnetization, and magnetic susceptibility are described by the critical exponents α, β, and γ. Determining these exponents in an MC simulation can be tricky since the results near a second order phase transition are strongly dependent on system size. However, a well-established technique known as finite size scaling allows one to extrapolate results for a series of small systems to the thermodynamic limit.

The project: Determine the above mentioned exponents (with error estimates) for the 2D and 3D Ising models. (See problem 17.10 in the handout for some details).

Project #2 (Andrew): Fluid Structure: Radial distribution function for a hard disk fluid

Although simple liquids lack any long range structure, they do display short range structure on a length scale of several molecular diameters. This structure is usually described in terms of the radial distribution function $g(r)$ [see Chapt. 7 of "Intro. to Modern Stat. Mech." by Chandler]. This radial distribution function can be measured indirectly via X-ray and neutron scattering experiments and it can be used to compute most thermodynamic properties of a liquid.

The project: Implement the algorithm described in Chandler Sec. 7.8 to compute $g(r)$ for a fluid of hard disks. Run simulations for a series of fluid densities, determining $g(r)$ in each case. Extrapolate the contact value of the radial distribution function $g(r\rightarrow\sigma)$ and thus determine the pressure of the hard disk fluid at each density (as described in Chandler Problems 7.33 and 7.34).

Project #3: Polymer Size: Scaling exponents for 2 and 3-dimensional self-avoiding walks

For certain conditions the dimensional properties of polymer molecules are well described by modeling the polymer as a self-avoiding walk. There are two common measures of the size of a polymer, the mean-square end-to-end distance $\langle r_{1N}^2\rangle$ and the radius of gyration $\langle R_g^2\rangle=\sum_{i<j}\langle r_{ij}^2\rangle/N^2$, where r_{ij} is the distance between sites i and j of the polymer. If the polymer were a simple random walk, either of these sizes ($\langle R^2\rangle$ for short) would scale as the length of the walk ($\langle R^2\rangle\sim N$). However, for a self-avoiding walk, overlapping configurations are prohibited which leads to the scaling behavior $\langle R^2\rangle\sim N^{2\nu}$ where 2ν is a "universal" scaling exponent ($2\nu>1$) which depends only on spatial dimension.

The project: Write a program that determines the equilibrium values of $\langle r_{1N}^2\rangle$ and $\langle R_g^2\rangle$ for a self-avoiding walk of length N on a lattice (I would recommend using the "pivot algorithm"). Determine the scaling exponent 2ν in both two and three dimensions (with error estimates). Possible extension: Add a nearest neighbor attractive potential to the model and study the variation of $\langle R^2\rangle$ with temperature.

Project #4 (Su & Christian): Cluster Growth Models: Fractal dimensions for compact and non-compact clusters

The growth of cell colonies and snowflakes can be described by two different simple growth algorithms. In the Eden model, one starts with a seed particle at the origin and randomly chooses a perimeter site to add the next particle. Repeated application of this growth rule leads to a compact cluster resembling a cell colony. In the diffusion limited aggregation (DLA) model, one starts with a seed particle at the origin and releases a "random walker" from a circular perimeter. When the walker arrives at a site adjacent to the seed, it becomes part of the cluster. Repeated application of this growth algorithm leads to a branched, non-compact cluster resembling a snowflake. To quantify the nature of these clusters one can measure their fractal dimension d_f defined by the relation $m(r) = Ar^{d_f}$ where $m(r)$ is the mass of the cluster contained within a radius r from the cluster center.

The project: Write programs for both the Eden and DLA cluster growth models on a lattice. In each case compute the fractal dimensions (with error estimates) of the resulting clusters. Do this first in 2D and then in 3D.