PH353, May 31, 2006
Ising model of a magnetic solid in 1 and 2 dimensions: Monte Carlo estimation.

In this lab we will use the Monte Carlo method to estimate the parameters (mean energy, heat capacity, magnetization and magnetic susceptibility) of a lattice of interacting dipoles. See the treatment from Koonin, *Computational Physics* for a complete description of the theoretical problem. A more limited treatment is found in Schroeder, Chapter 8.

Method: NxN lattices of spins are randomly generated according to the Boltzmann distribution. That is, the probability that an individual spin S_i points up or down depends on the state of its neighbors S_j and the presence of a magnetic field B. The lattice is assumed to be in contact with a "heat bath" of temperature T.

For an individual spin:

$$P(S_i) = (1/Z)\exp\left(\frac{-J\Sigma_{pairs} S_i S_j - \mu B \Sigma S_i}{kT}\right)$$

We don't know Z and can't calculate it. However, we can estimate it by generating a bunch of lattices L_i. Each of these lattices has energy E_i and magnetization M_i so we can calculate average values <E> and <M> by just averaging these from the generated lattices. In addition we can calculate the heat capacity and the magnetic susceptibility from the variances of these quantities.

$$C_B = (< E^2 > - < E >^2 / kT^2$$
$$\mathrm{X} = (< M^2 > - < M >^2) / kT^2$$

Here, we take k and μ to be equal to 1.0, so that only the ratios of J/T and/or B/T matter. The complete solution for an infinite lattice is given in Koonin, *Computational Physics*. The interesting feature of this model is that at low temperature, the lattice "freezes", that is, it becomes a ferromagnet. The critical temperature T_c in the above units is 2.269. Near this temperature, C_B and X peak. In fact, X is infinite at T_c for an infinite lattice, but in a finite lattice the singularity is removed.

Several programs are available for generating lattices and many are available on line. A nice Java version is available at http://stp.clarku.edu/simulations/ising2d/
However, this implementation is too slow for serious work, because you have to generate a *large number of lattices* and average over them in order to get reasonable results. A version written in QBASIC is available on the course web page, including an executable that should run on any PC. It is about 100 times faster than the Java version.

Instructions for Lab Assignment:

Using any of the available programs, first run the simulation at the critical temperature 2.269, for a 32x32 lattice with no applied magnetic field B. Observe the behavior. There are large fluctuations in the magnetization in both directions (i.e. nearly all "up" spins or nearly all "down" spins). Application of even a small B field will cause the lattice to magnetize nearly completely in the favored direction. Below T_c, the behavior will be uninteresting and mostly spin-aligned, but above T_c, the size of the magnetic domains will be reduced substantially and the overall fluctuations will diminish.

1. Turn off the spin-spin interaction by setting **J=0** (the only useful values of J are -1, 0 and 1). This models a lattice of non-interacting spins. For **B=1** and various values of T, verify that you get the theoretical result for the mean energy <E> and magnetization <M> as derived in class (with μ=1 and k=1):

$$< E >= -B \tanh\left(\frac{B}{T}\right)$$

$$< M >= -E / B$$

   Make a plot of the results.

2. Turn off B by setting **B=0** and set **J=1** (the spin-spin coupling). For lattice sizes of 8x8, 16x16 and 32x32, calculate and make plots of <E>, <M>, C_B and X for temperatures in the range 2-10, paying close attention to the behavior near Tc = 2.269 (i.e. try temperatures 2.1,2.2,2.3,2.4 etc.). **If your graphs of C_B and X are not smooth curves, you are not averaging over a large enough sample of lattices!**

3. Question: how does the lattice size affect the singularity in X and the width of C_B?

4. Experiment with **J=1** and several values of B to see the effect.

5. Simulate an antiferromagnet by setting J=-1. What is its behavior? Does it have a critical temperature? What is the behavior of the heat capacity C_B and the susceptibility X?

<u>Notes on using the QBASIC program ISING.BAS (or ISING.EXE).</u>

1. The program will ask for the number of "thermalization sweeps". This is because the initial lattice is a randomize collection of spins, not equilibrated at the heat bath temperature T. 100 thermalization sweeps should be enough to equilibrate the lattice, but you might experiment. Otherwise, your averages might include a highly improbable configuration, especially if T is low.
2. The program asks for number of passes and "sweeps per pass". The average values <E>, $<E^2>$, etc. are updated once each pass, but only after some number of thermalization sweeps so that the lattices tend not be be correlated with one another. You might try 1000 passes and 10 sweeps per pass initially, but this may not be good enough to get accurate values near T_c! Experiment with larger numbers for both keeping in mind that the number of lattices generated is (number of passes)x(sweeps per pass) so the computer time will go up accordingly.
3. The random number generator may be "seeded" differently to get a different series. Try seeds of 1, 3, 5, etc. to see if the averages change. If they do, **you aren't averaging over enough samples!**