Introduction to Modeling and Simulation, Spring 2002, MIT

1.992, 2.993, 3.04, 10.94, 18.996, 22.091

Problem Set 4 due on Wed March 13, 2002

Study qualitative behavior of the two-dimensional Ising model.

Write a computer program to simulate $L \times L$ two-dimensional Ising model in the absence of an external field. The energy of the system is given by

$$E = -J \sum_{\{i,j\}} s_i s_j$$

where the sum is over all nearest neighbors on the square lattice. Set $J = 1, k_B = 1$.

The total magnetization M of the system is

$$M = \sum_{i=1}^{L} s_i$$

Use Metropolis Monte Carlo algorithm to simulate dynamics of the system.

(**For extra credit:** use periodic boundary conditions and explain how you did this.)

If you can't program download the program *ising* from
`http://sip.clarku.edu/programs.html` `Chapter 17`.

1 For $L = 16$ and $T = 2$ determine the number of Monte Carlo steps n_{eq} needed to equilibrate the system. Start your simulations from a configuration where the direction of each spin is chosen at random. Plot the values of E and M after each Monte Carlo step *per spin* (Hint: after L^2 Metropolis tests).

2 Visualize the states of the spins at equilibrium and a few transitional time points. You can either use an external graphics program (MATLAB, Mathematica, etc) or just print out $L \times L$ table of spins. Is the system "disordered" at $T = 2$ after the equilibration is established.

3 Repeat 1 and 2 with all spins initially "up". Does the equilibration time increase or decrease? Do you see qualitative changes in the final configuration?

4 Repeat 1-3 for $T = 0.5$ and $T = 2$.

5 Starting your runs from all spins up, compute equilibrium average energy *per spin* $\langle E \rangle / L^2$ and average equilibrium magnetization *per spin* $m = \langle M \rangle / L^2$ for different temperatures T. Use at least 1000 Monte Carlo steps *per spin*. Plot vs T, vs T for $0.5 \leq T \leq 3.5$. Describe the behavior of the system in terms of order-disorder transition.

Homework (Leonid Mirny) on Monday at 2pm, Room 24-115. **Do not ...**