Computer Tutorial 2: Monte Carlo simulations of Ising Model

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November 6, 2010

Definition of the Ising Model:

- Set of Spins on a Lattice
- Each spin can be +1 or -1
- Only nearest neighbour interactions

$$H(\{S_i\}) = -J_{int} \sum_{<ij>} S_i S_j - H_{ext} \sum_i S_i$$

We will implement this in 2-D on an $N \times N$ lattice with Periodic Boundary Conditions.

Statitical Mechanics of the Ising Model:

- Partition function

$$Q = \sum_{States} \exp(-H(\{S_i\})/kT)$$

- Calculate averages over this Boltzmann distribution

$$\langle A \rangle = \sum_{j}^{Configurations} A_j \exp(-H(j)/kT)$$

- We need to generate these configurations

We will use a Metropolis scheme to generte these configurations

Sample MC Simulation:IsingMetropolis.c;

- Define State of system – Values of all spins and size of system Nx and Ny – Variable Spin[X][Y]
- Choose some initial condition (Randomly chosen)
- Trial Move – Pick a spin at random and flip it.
- Acceptance Ratio – According to Metropolis criteria

$$p_{acc}(a - - > b) = \mathrm{Min}(1, \exp(-\delta E / k_B T)$$

A sequence of such trial moves with this acceptance probability will attain the final equilibrium distribution of states.

Understanding

- Visually understanding - Look at Output file: vi Output
- Calculate the average magnetization
- Calculate T_c – Very difficult
- Estimate T_c

We have to do a lot more accurate calculations to get the critical temperature. Larger system, more trials, more averaging.
Try to modify IsingMetropolis.h to see if all our intuition works.

Implementation of IsingMetropolis.c

- Edit the header file IsingMetropolis.h
- Compile : gcc -lm IsingMetropolis.c -o IsingMetropolis
- Run: ./IsingMetropolis
- View Output: vi Output

Future work: Try to calculate ensemble averages by averaging magnetization over a longer production period.