

Topic 3: Monte Carlo Simulation of Magnetic Materials (continued)

The program `ising.c` implements a serial version of the Metropolis Monte Carlo algorithm applied to the 2-D Ising Model on an $L \times L$ square lattice.

One Monte Carlo step consists of applying the Metropolis algorithm to N spins, either by *sweeping* the lattice, or by choosing N spins at random. This is done to reduce correlations between successive configurations. If the Metropolis algorithm were applied only to one spin, all the others would remain unchanged and the two successive configurations would be almost identical!

```
for (x = 0; x < L; x++) {
    for (y = 0; y < L; y++) {
        sum_of_neighbors = spin[x][next[y]] + spin[x][prev[y]]
            + spin[next[x]][y] + spin[prev[x]][y];
        delta_SS = 2 * spin[x][y] * sum_of_neighbors;
        ratio_of_Boltzmann_factors = w[delta_SS + 8][spin[x][y] + 1];
        if (qad_rand(0) < ratio_of_Boltzmann_factors) {
            spin[x][y] = -spin[x][y];
            M += 2 * spin[x][y];
            SS -= delta_SS;
            ++flips;
        }
    }
}
```

This double loop has been optimized in two ways:

Periodic Boundary Conditions: The indices of neighboring spins are stored in two arrays `next` and `prev` which are initialized as follows:

```
for (i = 0; i < L; i++) {
    next[i] = i + 1;
    prev[i] = i - 1;
}
next[L - 1] = 0;
prev[0] = L - 1;
```

Computation of Boltzmann Factors: This is potentially very time-consuming because the evaluation of a floating point exponential typically takes several machine cycles. However, it turns out that for given T and H , there are only 10 distinct values for the change in energy due to a trial Metropolis spin flip $s_i \rightarrow -s_i$:

$$\Delta E = E_{\text{trial}} - E = 2s_i \left[J \left(\sum_{\text{neighbors } j} s_j \right) + H \right].$$

This is because s_i can take two values ± 1 , and the sum of the 4 neighboring spins can take 5 different values:

1. +4 if all neighbors are “up” ,
2. +2 if 3 neighbors are “up” and the fourth “down” ,

3. 0 if 2 are “up” and the other two “down”,
4. -2 if 3 are “down” and the fourth “up”,
5. $+4$ if all neighbors are “down”.

These exponential values can be computed and stored in an array $w[][]$ before the simulation begins:

```
for (i = -8; i <= 8; i += 4) {  
    w[i + 8][0] = exp( - (i * J + 2 * H) / T);  
    w[i + 8][2] = exp( - (i * J - 2 * H) / T);  
}
```

This array is indexed by the integers $8 + 2s_i \times \sum_{\text{neighbors } j} s_j$ and $1 + s_i$ as shown in the code fragment.

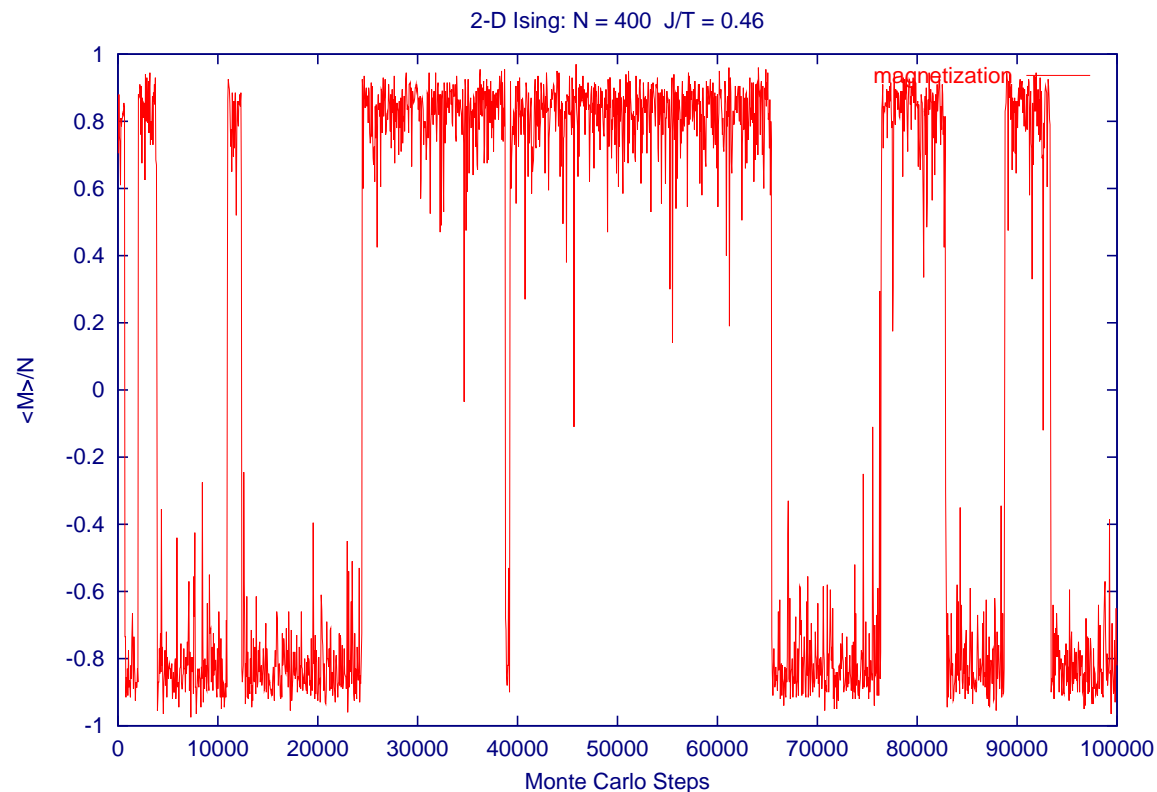
The program is otherwise fairly straightforward:

- The spins are initialized either to a *cold start* in which all the spins point up as appropriate to $T = 0$, or a *hot start* in which the spins are chosen randomly up or down as appropriate to $T = \infty$.
- A number of thermalization steps are taken to allow the system to come to thermal equilibrium at the specified temperature.

- The production steps are binned into blocks and average values of the magnetization and energy computed in each block so as to estimate the Monte Carlo errors in two different ways.

Behavior of the Magnetization

The following figure shows the measured magnetization as a function of Monte Carlo step.



Note that the magnetization $M = \sum_i s_i$ per spin fluctuates between values $\approx \pm 0.8$ at this temperature. Thus the system behaves like a magnet, but one in which the north and south poles spontaneously flip as a function of “Monte Carlo time”. This means that the average magnetization $\langle M \rangle = \langle \sum_i s_i \rangle = 0$ if the simulation is run for a sufficiently long time!

In fact it is easy to see that

$$\langle M \rangle = \frac{\sum_{\text{configs}} M e^{-E/k_B T}}{\sum_{\text{configs}} e^{-E/k_B T}} = 0, \quad \text{if } H = 0.$$

This is because the energy $E = -J \sum s_i s_j$ does not change if we flip all spins $s_i \rightarrow -s_i$, while the magnetization changes sign. The sum over configurations of course does not change because we simply sum over $s_i = \mp 1$ instead of $s_i = \pm 1$. Thus

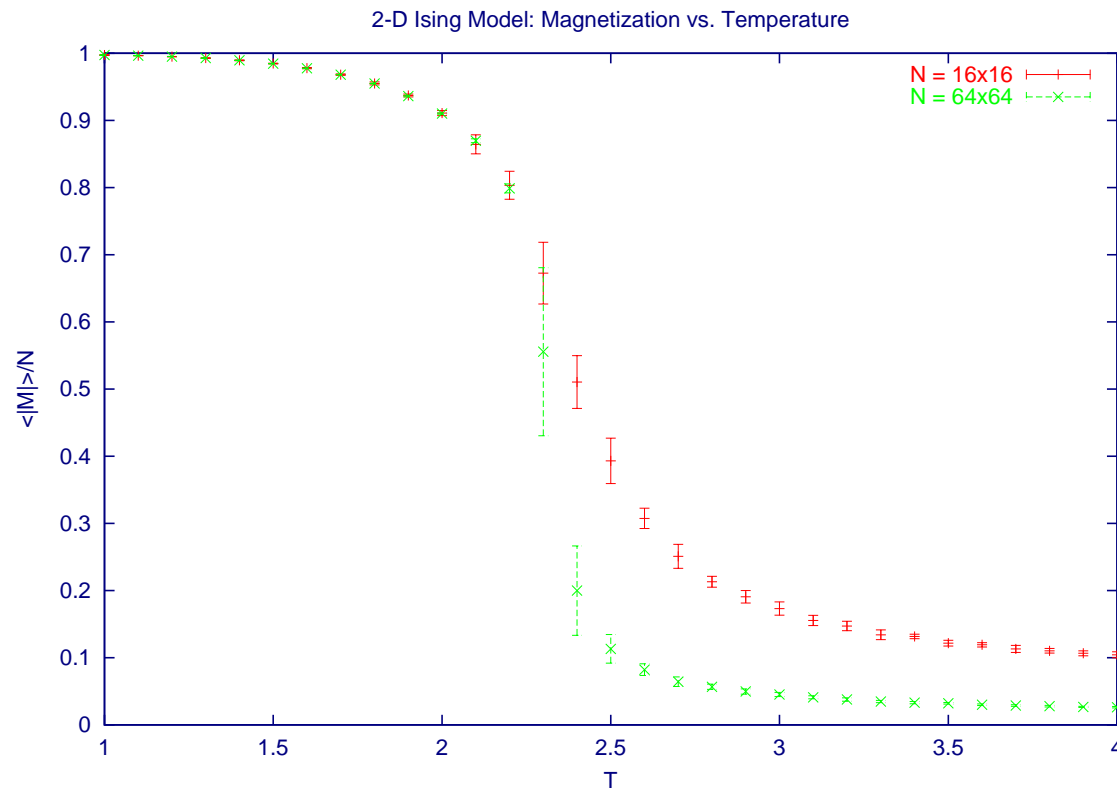
$$\langle M \rangle = -\langle M \rangle \quad \Rightarrow \quad 2\langle M \rangle = 0.$$

How then can a permanent magnet exist? The answer is that true ferromagnetism can only occur in the thermodynamic limit of an infinite number of spins. In this limit it is possible for the spin-flip symmetry to be *spontaneously broken*. In a finite permanent magnet of finite size, it is in fact possible for the north and south poles to reverse spontaneously: however, it can be shown that the time between such spontaneous reversals is astronomically large for any macroscopic magnet.

To detect the presence of ferromagnetism in a Monte Carlo simulation, it is therefore necessary to measure $\langle |M| \rangle$.

Simulating the Ferromagnetic-Paramagnetic Phase Transition

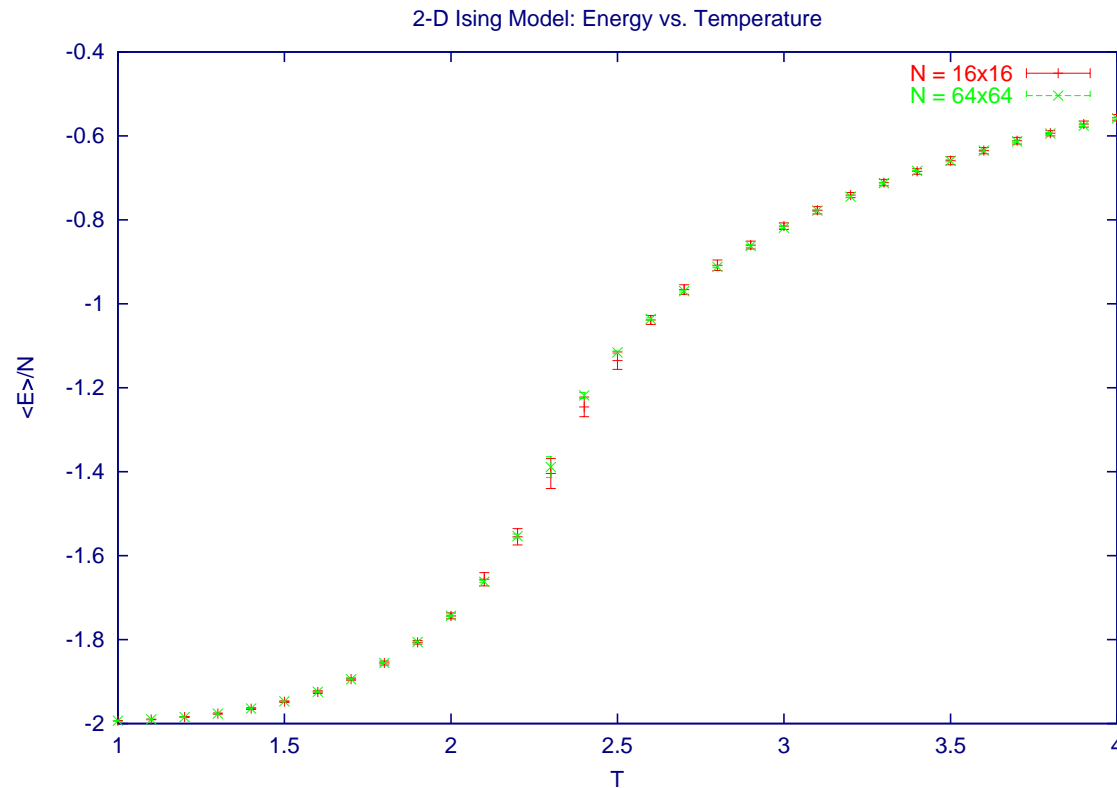
The properties of the Ising Model can be measured as a function of temperature T .



The figure shows the average value of the the magnitude of the magnetization per spin plotted vs. temperature. The data were obtained using 10,000 Monte Carlo steps at each value of T . The error bars were computed by binning the data in 20 blocks of 500 Monte Carlo steps each. Notice the following:

- There is a definite change from ferromagnetic to paramagnetic behavior at $T \approx 2.3$. It can be shown theoretically that the Curie temperature for this model in the thermodynamic limit $N \rightarrow \infty$ is $T_c \simeq 2.269$. The measured transition temperature is greater than the theoretical value: this is due to use of periodic boundary conditions; with free boundary conditions the measured transition is below the theoretical value.
- The error bars get larger in the region of this phase transition. This indicates that thermal fluctuations in the system are larger in the critical region. It can be shown theoretically that the *correlation length* for fluctuations in the system increases as T approaches T_c from above or below.
- Comparing systems with different numbers of spins, $N = 16 \times 16$ and $N = 64 \times 64$:
 - The transition region becomes narrower as the number of spins N increases.
 - The fluctuations become larger as N increases. It can be shown theoretically that the correlation length becomes infinite at $T = T_c$ in the *thermodynamic limit*, i.e., as $N \rightarrow \infty$.
 - The location of the transition moves closer to the theoretical value $T_c = 2.267$ as N increases.

The following figure shows the behavior of the average energy per spin as a function of temperature. This curve is *sigmoidal* (S-shaped), with the point of inflection close to the theoretical value of $T_c = 2.267$.



The measurements show that the energy is less sensitive to critical fluctuations than the magnetization. The error bars are smaller in general, and increasing the number of spins from $16 \times 16 = 256$ to $64 \times 64 = 4096$ does not appreciably change the curve or the error bars.

It can be shown theoretically that the fluctuations in the magnetization, *the isothermal susceptibility*, diverges like

$$\chi_T \sim \frac{1}{|T - T_c|^{\frac{7}{4}}},$$

for the 2-D Ising model, while the fluctuations in the energy, *the heat capacity at constant H* , has a much milder divergence

$$C_H \sim \log \left(\frac{1}{|T - T_c|} \right) .$$