Project B: Thermodynamic Simulations using the Ising Model

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Abstract

The Ising model allows to illustrate the behaviour of the spins in a ferromagnetic material with a representation of the system by a two-dimensional lattice of spins up and down. The theory predicts that the spins tend to align at low temperatures and that they spin up and down randomly at high temperature. There is thus a phase transition defined by the Curie temperature. These expectations are confirmed by using the Monte Carlo method. For the first part of the experiment, we only consider the internal interactions, the results are consistent with the theory. Then, a magnetic field is applied. The spins tend to align with the field when the temperature is higher than the Curie Temperature, however this effect is not very significant at very high temperature because the thermal agitations dominate. For T less than T_c, the alignment of the spins by the magnetic field is only possible if the field is strong enough.

1 Introduction

In ordinary materials, the associated magnetic dipoles of the atoms have a randomized orientations, which means that the overall distribution would results in no overall macroscopic magnetic moment. But, in some cases, magnetic moments are produced due to a preferred alignment of the atomic spins.

This is due to the Energy minimization and Entropy maximization. These principles are important in moderating the overall effect with the temperature as an important parameter. These behaviors are essentially encapsulated by the Gibbs distribution, i.e the probability that the system is in the α_j configuration is given by:

$$P(\alpha_j) = \frac{exp(E(\alpha)\beta)}{Z} \tag{1}$$

where $\beta = \frac{J}{kT}$ and Z is the partition function.

The quantities that describe the equilibrium of the system can be represented with these quantities.
1. Magnetisation

$$M = N^{-2} \sum_k \boldsymbol{S_k} \tag{2}$$

2. Heat Capacity

$$C = N^{-2}(kT)^{-2}(< E^2 > - < E >^2) \tag{3}$$

where it is linked to the variance of the energy

3. Susceptibility

$$\chi = N^{-2}J(kT)^{-1}(< S^2 > - < S >^2) \tag{4}$$

where $S = \sum \boldsymbol{S_k}$ and it is linked to the variance of the magnetisation

2 Method

2.1 Presentation of the Ising Model

The Ising model is a simple and mathematically tractable model that simplifies the complexity of the problem while retaining most of the essential physics. The model considers the problem by placing the dipole spins at regular lattice points and restricts the spin to be either up or down. In its simplest form, the interaction range amongst the dipoles is restricted to immediately adjacent sites(Nearest Neighbours). This produces a Hamiltonian for the system to be

$$E = -\frac{1}{2} \sum_{i,j} J_{i,j} \boldsymbol{S_i}.\boldsymbol{S_j} - \mu \sum_k \boldsymbol{S_k}.\boldsymbol{B} \tag{5}$$

where $\boldsymbol{S_i}$ is the spin of the ith site (either 1 or -1), J the interaction energy, μ the Bohr Magneton and $\boldsymbol{B}$ the applied magnetic field.

To maximize the interaction of the spins at the edges of the lattice, the periodic boundary condition is applied so the spins at the edges of the lattice

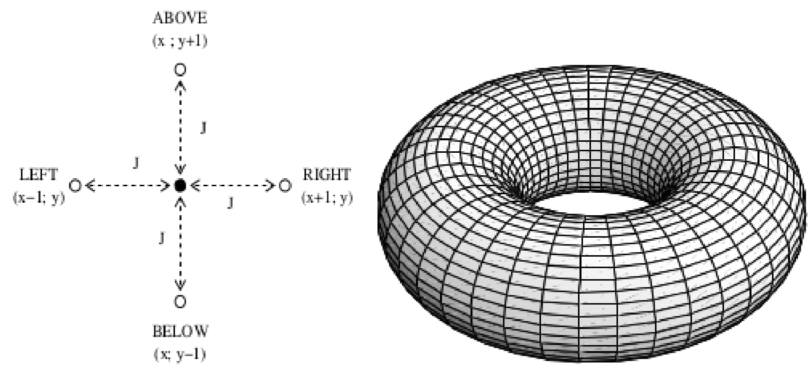

Figure 1: The figure on the left shows the neighbours'interaction and the torus on the right gives a pictorial representation of the boundary conditions

are made to interact with spins at the opposite edges. This can be visualized if we consider the 2D lattice being folded into a 3D torus with spins on the surface of the structure as shown in Figure 1.

2.2 Metropolis Algorithm

The use of the Ising Model meant that we can anticipate the parameter of the system by following the energy of each state. However, for a system with N spins, this immediately lead to a 2^N problem. By considering the equation of energy and magnetization more closely ; it is apparent that by checking every states of the system, we would waste so much effort in calculating improbable results. Thus, a better numerical sampling of the Metropolis Algorithm is used. That is if $\delta E < 0$, then flip the spin and if $\delta E > 0$ then flip the spin according to the Boltzmann probability.

The Metropolis method consists of a random sampling for a spin to flip. The chosen spin is flipped if it is energetically favourable. This is particularly desirable method as the system has at least 2^N configurations and the Metropolis Algorithm allows to us to reach equilibrium without having to test all of the configurations. This is due to the use of the Boltzmann distribution, we are maximising the entropy and thus reducing the free energy of the system.

2.3 Implementation

The 100×100 array is initialised at a low temperature configuration such that the spins are aligned or at a high temperature configuration with randomized spins of up or down. Then, the evolution at a given temperature is achieved by using the Metropolis Algorithm which ensures the system obey the Boltzmann distribution. To obtain a high accuracy on the transition value, we vary the β by 0.001 at each step. When the energy becomes stable and the system reaches an equilibrium, several variables like the heat capacity, the susceptibility and the magnetisation are calculated to observe the evolution of the system with β ranging from 0.1 to 1. For a given β, the starting lattice is defined as the stable lattice of the previous β. This is repeated in the scenario under a magnetic field.

3 Theoretical behaviour

1. At low temperatures, the interaction between the spins are strong so the spins tend to align with their neighbours. In this case, the magnetization reaches its maximal value $M = 1$. The magnetisation exists even if there is no external magnetic field.
2. At high temperature, the interaction is weak, the spins should be randomly distributed of up or down. So, the Magnetisation is close to 0. The system is metastable.
3. There exists a phase transition. In zero magnetic field, the critical temperature is the Curie Temperature

$$T_c = \frac{2}{ln(1+\sqrt{2})} \tag{6}$$

obtained using the Onsager's theory. According to the transition theory, the 2nd Order derivative of the Free energy in B and T are discontinuous at the transition phase. And since the susceptibility and the heat capacity are expressed with these derivatives, they should diverge at the critical temperature.

4 Result and Discussion

4.1 Cases of zero external magnetic field

4.1.1 Thermodynamic quantities against the temperature

We obtain a transition phase at a critical temperature $T = T_c$ which marks the demagnetisation. We notice a larger fluctuation as we approach the critical temperature because at T_c, spins start to compete with spins flipping. This causes significant changes in E and S.

From Figure 3, we find that the heat capacity peaks at around 0.27 ± 0.01 which agrees with the theoretical value.

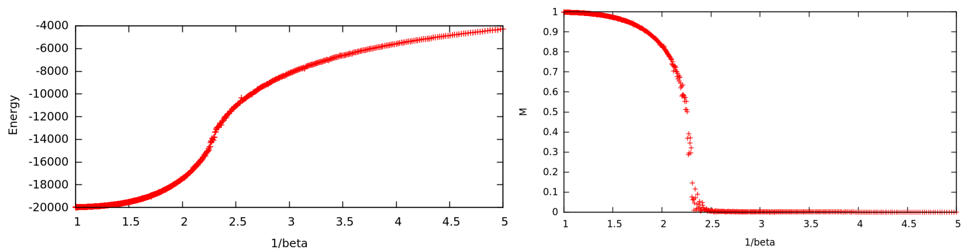

Figure 2: Case of zero external field with a lattice 100×100. On the right: Energy, in J-unity, against the temperature. At very low temperature, the energy is minimum and it slowly increases with the temperature. At the region close to the critical temperature, the slope becomes abrupt and the energy quickly decreases. This region is close to the Curie temperature. On the left, it is the magnetisation against the temperature. The magnetisation is approximately one at low temperature and above the transition temperature, the magnetisation is zero

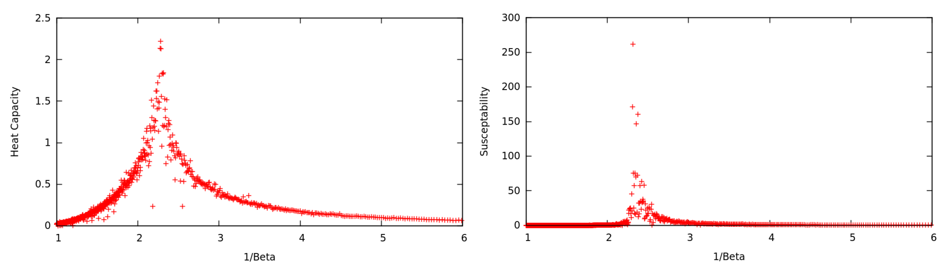

Figure 3: In the case of zero external field with a lattice of 100× 100. On the right, the heat capacity , again in J-unity, against the temperature. The capacity has a peak at $T \approx 2.27 \pm 0.01$ which symbolises the phase transition and it decreases to zero at higher temperature. On the left, the susceptibility shows a more abrupt peak as well but at $T \approx 2.31 \pm 0.01$, the susceptibility again decrease to zero at higher temperatures

Generally, we have observed the following results in our simulations:

- At $\beta = 1$, at a very low temperature, the spins are fully aligned with the magnetisation is maximum. The spins are gradually thermalized as the temperature increases.

- At β is close to T_c, there are several clusters of aligned spins, in each cluster the magnetisation is maximum but the magnetisation of the set is zero overall because the probability to be in the configuration α_j is equal to the probability to be in the configuration $-\alpha_j$. T_c marks the transition from an ordered set of lattice into an disordered set of lattice.

- At very high temperature ($\beta = 0$), the dipoles are randomly oriented.

We find that the susceptibility peaks at around $T \approx 2.3 \pm 0.01$, which is different for the value obtained using the heat capacity. This may be due to the subtle fact that our lattice are finite in nature and this has an implication.

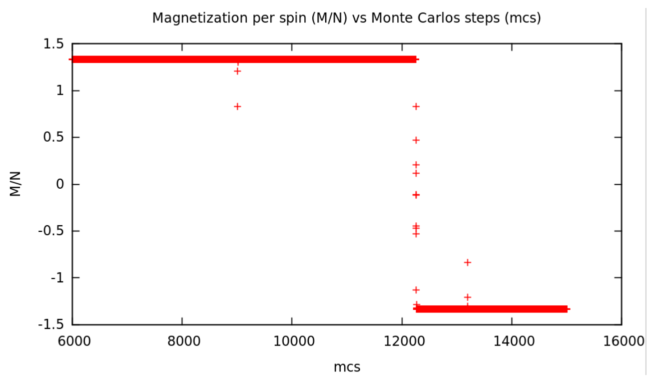

Figure 4: This is Magnetization per spin vs Monte Carlo steps at $T = 1$ for an 2×2 array. It is unphysical that the system to completely flip its spins, but this is due to the finite nature of our array.

Figure 4 shows that although the system is well below the Curie temperature and should be very stable, but there is always a finite probability for the system to experience a complete flip of magnetization. This thus has an effect for the variance of magnetisation and thus the susceptibility at T_c. Using the fact that the probability of the states to be symmetric, that is $P(\alpha) = P(-\alpha)$. This means if we use the $< abs(M) >$ instead of just $< M >$, this should give a better value for the susceptibility. You might suspect that this could be wrong as this woud give a non-zero value of Magnetsation at $T > T_c$. But since T_c marks between the region of spins flipping and the region of stable spins, the susceptibility graph should peak at a more corrected T_c. However, this effect should be small at a big lattice.

4.1.2 Finite lattice effect

To further illustrate the effect of the finite nature of the lattice on the transition phase, the thermodynamics quantities are plotted for several sizes. We can clearly see that as the lattice size gets bigger, the phase transition can be shown more clearly.

Figure 5 shows very beautifully that the shape of the gradient becomes more distinct as the lattice size is increased and there are far more apparent features that the larger lattice produces in the curve and illustrates a more apparent phase transition. It is however clear that there is no divergence but merely a progressive steepening of the peak as N increases. The point in which the plot is peaked should be noted as a possible point of divergence. We also notice that statistical fluctuations are a lot less with bigger lattices. As this computation involves a lot of random sampling; increasing the size of the lattice gives better statistics.

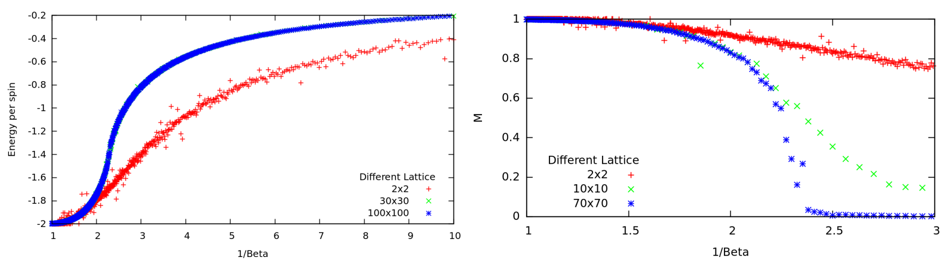

Figure 5: On the top: Energy per spin against the temperature at different lattice size. As the lattice size increases, we see a more abrupt change in energy. On the bottom: Magnetisation at different lattice size. The behaviour for the three lines are similar but there is definitely a faster demagnetisation at bigger lattice. It is also interesting to see that demagnetisation is not completed at smaller lattice and the M is at a constant value even at a high temperature.

4.1.3 Exact Results

Using a 2x2 array, there are 2^4 configurations that can be reduced to 4 by symmetric considerations. Configuration A is the fully aligned spin and configuration B has one spin in the opposite direction to the other three while C and D has two spins up and two spins down. And the exact equations is as follows:

$$Z = 2e^{8\beta} + 12 + 2e^{-8\beta} \tag{7}$$

$$< E >= -\frac{1}{Z}[2(8)e^{8\beta} + 2(-8)e^{-8\beta}] \tag{8}$$

$$< E^2 >= -\frac{1}{Z}[2(64)e^{8\beta} + 2(64)e^{-8\beta}] \tag{9}$$

$$< |M| >= \frac{1}{Z}2(4)e8\beta + 8(2) \tag{10}$$

$$< M^2 >= \frac{1}{Z}2(16)e8\beta + 8(4) \tag{11}$$

Applying the above equations, we can obtain the heat capacity and susceptibility. The comparison of these results are shown in Figure 6. The results achieved by the Monte Carlo method match the exact calculation exceptionally well. Slight deviations occur at phase transition.

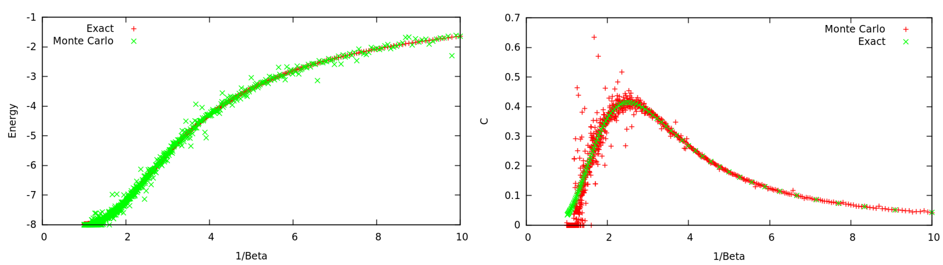

Figure 6: This is an 2×2 array's Monte Carlo result and the exact analytical result. On the left, we have the usual Energy vs 1/Beta plot. On the right, we have the Heat Capacity vs 1/Beta plot. Using only a 2×2 Ising, we can already see that the Monte Carlo method works surprisingly well.

4.2 Case with an external B field

In the latter part of the computations, we inserts an external magnetic field in the lattice. As we apply the field, the peaks of C and χ are shifted to higher temperatures and their magnitudes are reduced with χ being more sensitive to the field. We also see more alignments of spins to the external field and the symmetry of spin is broken, thus the domain do not compete but instead align itself accordingly. At higher temperature, thermal process dominate over μB.

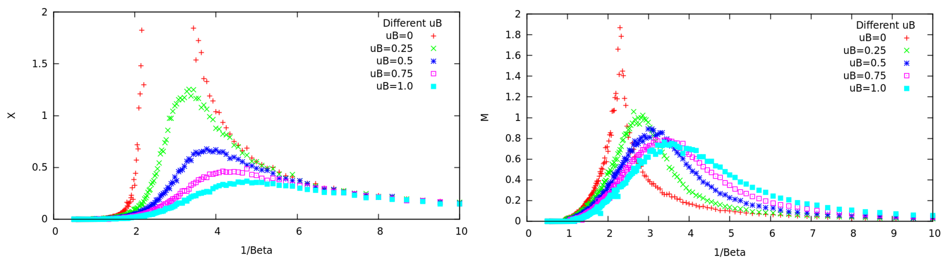

Figure 7: This is a 50×50 Ising model under an influence of an external magnetic field with at different β. The temperature at which there is a peak, is slightly displaced toward the bigger values.On the right: Influence of the magnetic field on the susceptibility with a lattice 50 × 50. The magnetic field generates an decreasing of the magnitude of the peak. At high temperature, the magnetic field has almost no effect. The thermal agitation makes negligible the effect of the magnetic field.

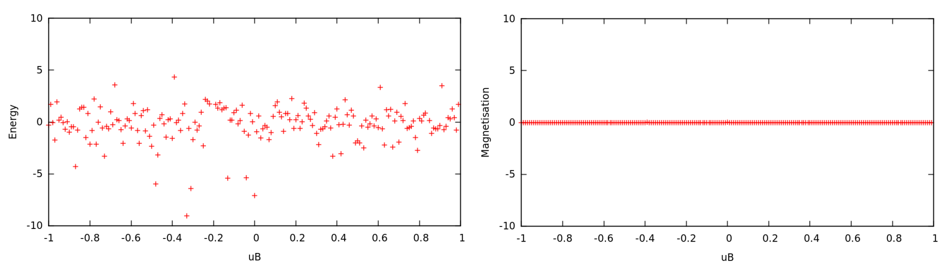

Figure 8: This is a 50×50 Ising model under an influence of an external magnetic field with $\beta = 0$(At a very high temperature). The magnetic field can not establish an order, the temperature is much too high, it confirms the previous results about thermal agitation dominates over the μB influence

The spins tends to align to the magnetic field at low temperature but has minimal effect at higher temperature. We see that there are discontinuity in the magnetisation at low temperature.

By changing the μB from $-1J$ to $1J$, the results are interesting for the cases when $T < T_c$ (Figure 9 and 10). When the starting magnetic field is a large positive value. The magnetisation is positive and thus align with B. As B goes down, the energy linearly increases with μB. The magnetisation is constant until a critical value of B_c, where it discontinuously flipped to negative and linearly decreases with μB. This dynamic is exactly the same when the starting magnetic field is negative with a negative B_c. The value of B_c varies with β.

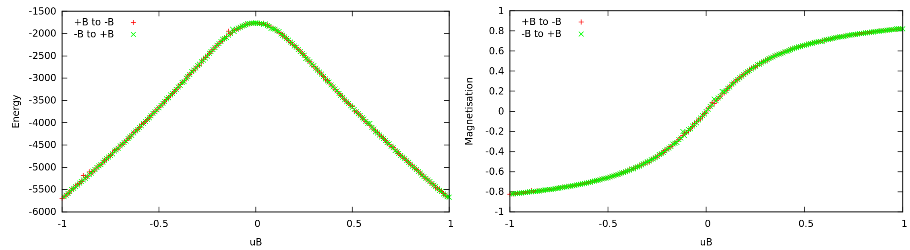

Figure 9: This is a 50x50 Ising model under an influence of an external magnetic field with $\beta = 0.3$ On the left: Energy against the magnetic field. On the right: Magnetisation against the magnetic field. At the beginning, the magnetic field has a large positive value, the magnetisation is positive and maximum, the spins are thus up, they align with the magnetic field. Then the energy linearly increases with uB until the sign of the magnetic field changes. The magnetisation becomes negative. The spins tend to align with the magnetic field and the energy linearly decrease with μB.

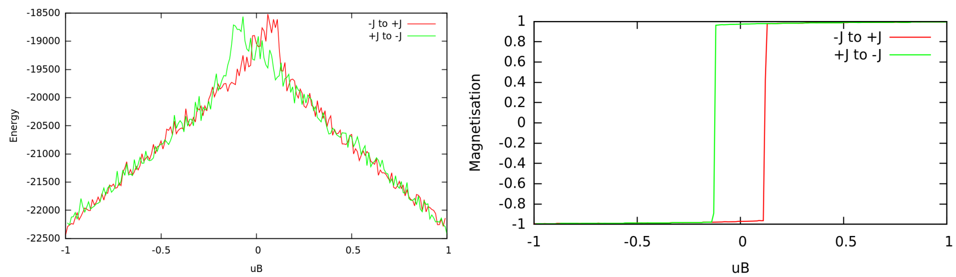

Figure 10: This is a 50x50 Ising model under an influence of an external magnetic field with $\beta = 0.6$ On the left: Energy against the magnetic field. On the right: Magnetisation against the magnetic field.

Since the spins are initially aligned with the field, as the B field decreases, the spins alignment still retains and hence the magnetisation is memorised(the configuration is frozen) until it goes to a point where all spins are forced to align in the opposite direction. This results in an instantaneous change in magnetisation. This agrees with the theoretical behaviour that when a ferromagnet is magnetised in one direction, removing B will not demagnetise the magnet but instead by applying an opposite B to demagnetise it. This property is useful for storing information. This is fundamentally manifested from the nearest neighbour interaction which is a local property, but has drastic macroscopic consequences.

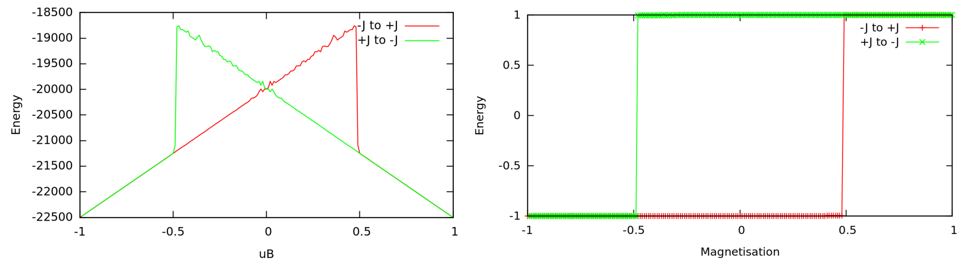

Figure 11: This is a 50x50 Ising model under an influence of an external magnetic field with $\beta = 1.0$ On the left: Energy against the magnetic field. On the right: Magnetisation against the magnetic field.

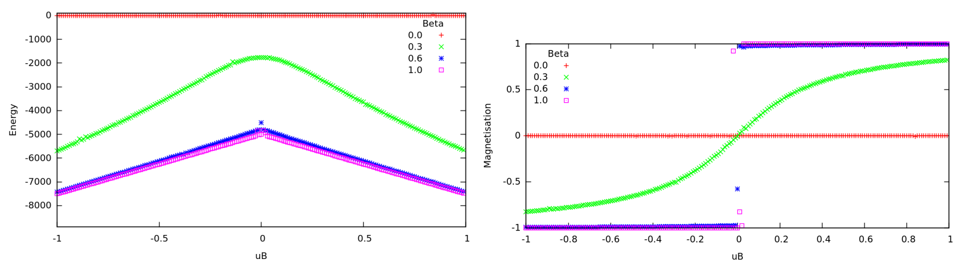

Figure 12: This is a 50×50 Ising model under influence of a magnetic field under different temperatures. This is obtained by initiating the array of spins in randomized configuration at each μB. By doing this, we effectively destroy the memory of the configuration and therefore the sysmetry in our results. On the left: Energy against the magnetic field. On the right: Magnetisation against the magnetic field. We can see energy value is highest when $B = 0$

4.3 Conclusion

The Monte Carlo method applied on the Ising Model allows us to obtain thermodynamic quantities evolutions. The results are consistent with the theoretical behaviour and expected values. By using a large enough lattice, we are able to minimize much of the finite size effect.

In the cases without a magnetic field, we see a strong evidence of a phase transition at the critical temperature. This transition separates $T < T_c$, where the magnetisation is maximum with the spins aligned, and $T > T_c$, where the magnetisation is zero with the spins randomly orientated.

In the presence of a magnetic field, the phase transition is less obvious. At a very high temperature, the field has almost no effect as the thermal agitation dominates the system. Nonetheless, the spins generally align with the magnetic field at low temperature. At T is close to T_c, the alignment of spins happens only if the field is above a certain value.

Furthermore, we could find a better value of T_c for an infinitely large grid by finding the relationship between lattice size N and the critical temperature. The relationship can be approximated by extrapolating N to infinity and thus finding a better value of T_c.

Other algorithms can be used to investigate the critical region of the Ising model such as the Wolff Algorithm.

5 Reference

1. Monte Carlo Methods in Statistical Physics, Newman and Barkema

2. Monte Carlo Methods in Statistical Physics, Binder and Heermann

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6 Acknowledgment

Thanks for the help from the demonstrators, it would have been impossible without them. And as some of the simulations took days to run, I also want to thanks the HPC department for letting me run the simulations at theirs again.