Phase transitions in magnetic systems

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Abstract

In this work we use Monte Carlo simulations with the Metropolis algorithm to study the 2-dimensional Ising model for finite and infinite spin sites, using lattice sizes up to 100×100. The purpose is to understand Monte Carlo simulations and parallellization of code, and to compare numerically computed values with analytical values. We find a simulated estimated critical temperature in the infinite lattice limit of $\frac{k_B T}{J} = 2.273$, agreeing with the analytic value to 3 significant digits. Our computed values for the 2×2 lattice agree with analytical values of expected energy and absolute magnetization to 4 significant digits at 10^6 Monte Carlo cycles, the magnetic susceptibility to 3 significant digits, while the heat capacity agrees to 1 significant digit. We find that running simulations on multiple cores in parallel could increase performance by a factor of 2. The accuracy of the critical temperature could be improved by increasing both the number of Monte Carlo cycles and the resolution of the temperature, to more accurately resolve the critical temperature for each of the four lattices and to then estimate the infinite limit more precisely.

1 Introduction

The Ising model [1] represents one of the simplest, yet most frequently studied models of ferromagnetism in statistical mechanics. Despite the simplicity and the fact that the model was originally proposed for a theoretical description of insulating magnetic materials, the Ising model and its variants have an extraordinary capability of elucidating co-operative phenomena of seemingly diverse physical origin. Apart from the traditional applications in magnetism, the Ising-like models have also found manifold applications from seemingly diverse research areas [2] such as: biophysics [3], [4], neuroscience, medicine [5], linguistic change of language [6], electronics and socio-economics [6]. The aforementioned list of applications is far from complete, but it demonstrates the versatility and the importance of the Ising-like models in modern science

In this work, we will confine ourselves to the study of phase transitions in a magnetic system for different lattice sizes and temperatures. Calculating expressions for the expectation values of physical parameters like the energy and magnetization of a thermodynamic system quickly gets computationally heavy due to high number of possible spin configurations. This problem is tackled by using the Monte Carlo based Metropolis algorithm for sampling the probability distribution of the system. With this method, we can simulate the system accurately and calculate the physical observables of interest, while avoiding the numerically toughest calculations.

We begin by benchmarking our algorithm with analytical results for a 2×2 lattice. Then, we increase the system to a 20×20 lattice, and estimate the time it takes to reach equilibrium. We also study various parameters such as the number of accepted

spin configurations and the energy distribution as function of temperature. The final purpose is to estimate the critical temperature of an infinite 2-dimensional spin lattice, and compare with the analytic result from Onsager [7]. This is done by extending to 40×40, 60×60, 80×80 and 100×100 lattice spin sites, and then using a Monte Carlo simulation to estimate the critical temperature for these lattice sizes.

The organization of this report is as follows. First, we review some important concepts in statistical mechanics, before explaining the key aspects of the implemented algorithm. Thereafter we present our results for the Monte Carlo simulations, beginning with the smaller lattices and using the knowledge gleaned to tune the simulations for larger lattices, and ending with a plot of the critical temperature for the larger lattices.

2 Theory

2.1 Boltzmann statistics

To derive macroscopic systems, and understand the behaviour of many-particle systems, we model the system statistically. In statistical mechanics we use probability models and microscopic physical laws. The probability distribution of a micro state i is given by the Boltzmann distribution

$$P_i = \frac{1}{Z} e^{-E_i \beta}, \tag{1}$$

where E_i is the energy, $\beta = \frac{1}{k_B T}$ and Z is the partition function, acting as a normalization factor, given by

$$Z = \sum_i e^{-\beta E_i}. \tag{2}$$

We use the probability of measuring a given state i (equation (1)) to calculate the expectation value of the energy, E and the magnetization, M.

$$\langle E \rangle = \frac{1}{Z} \sum_i E_i e^{-E_i \beta} \tag{3}$$

$$\langle M \rangle = \frac{1}{Z} \sum_i M_i e^{-E_i \beta} \tag{4}$$

From these expressions we can derive other physical properties such as the heat capacity at constant volume C_V given by

$$C_V = \frac{1}{k_B T^2} \left(\langle E \rangle^2 - \langle E^2 \rangle \right). \tag{5}$$

equation (5) describes the amount of energy needed to change the temperature.

We can find the magnetic susceptibility, χ, in the same manner, we get

$$\chi = \frac{1}{k_B T} \left(\langle M \rangle^2 - \langle M^2 \rangle \right). \tag{6}$$

The magnetic susceptibility tells us whether the material is attracted into, or repelled out of a magnetic field.

2.2 The Ising model

A popular model to simulate phase transitions, is the so-called Ising model. In one and two dimensions the Ising model has analytical solutions to several expectation values. The 2-dimensional Ising model for a square lattice in the absence of an external magnetic field is modelled as

$$H = -J \sum_{<ij>} s_i s_j, \tag{7}$$

where H is the total energy of the system, J is the coupling constant expressing the strength of the interaction between neighboring spins and the sum describes the spin-spin interaction between the nearest neighbours only. The spins can be either up or down, which we write $s_i = \pm 1$. We assume ferromagnetic ordering ($J > 0$), which makes it energetically favorable for neighboring spins to align – leading to spontaneous magnetization at low temperatures, T.

2.3 Phase transitions

A power law behavior can characterize the behavior of many physical quantities near the critical temperature T_C. For example, the mean magnetization for the Ising class of models is given by

$$\langle M(T) \rangle \sim (T - T_C)^{\beta}, \tag{8}$$

where $\beta = 1/8$ is the critical exponent. A similar relation is found for the heat capacity

$$C_v(T) \sim |T_C - T|^{\alpha}, \tag{9}$$

and the magnetic susceptibility

$$\chi(T) \sim |T_C - T|^{\gamma} \tag{10}$$

with critical components $\alpha = 0$ and $\gamma = 7/4$. Another important quantity is the correlation length, which also has a power law behaviour given by,

$$\xi = |T_C - T|^{-\nu}. \tag{11}$$

The correlation length is expected to be of the order of the lattice spacing for $T >> T_C$. The correlation length increases as we get closer to the critical temperature, because the spins become more and more correlated as T approaches T_C. For a finite lattice

size L, the correlation length can be shown to be proportional to L by the following relations

$$\begin{aligned} \langle M \rangle &\propto L^{-\beta/\nu} \\ C_V &\propto L^{\alpha/\nu} \\ \chi &\propto L^{\gamma/\nu}. \end{aligned} \tag{12}$$

Through so-called finite size scaling relations it is possible to relate the behavior at finite lattices with the results for an infinitely large lattice. The critical temperature scales then as

$$T_C(L = \infty) = T_C(L) - aL^{-1/\nu}, \tag{13}$$

where a is a constant and ν is defined in equation (11).

To estimate the constant a, one can compare the results of two lattices $T_C(L_1)$ and $T_C(L_2)$ by

$$(T_C(L_1) - aL_1^{-1/\nu}) - (T_C(L_2) - aL_2^{-1/\nu}) = a(L_1^{-1/\nu} - L_2^{-1/\nu}), \tag{14}$$

which gives the expression of a as

$$a = \frac{T_C(L_1) - T_C(L_2)}{L_1^{-1/\nu} - L_2^{-1/\nu}}. \tag{15}$$

Lars Onsager, the Norwegian born chemist and physicists was the first to solve the Ising model analytically in two dimensions for a general lattice size L [7]. From his work, we have that the analytical critical temperature in the thermodynamic limit is

$$k_B T_C/J = 2/\ln(1 + \sqrt{2}) \approx 2.269, \tag{16}$$

and the parameter $\nu = 1$.

2.4 Markov chains

A Markov chain takes a state 1 and generates a new state 2 with a *transition probability* $P(1 \to 2)$, and is a good description of a system that moves towards a steady state given an initial configuration. The transition probabilities needs to be time-independent and $P(1 \to 2)$ should only depend on the states 1 and 2, and is thus also independent of the system's time evolution. Further, the Markov chain must put the system in some state 2 when presented with the state 1. Mathematically this can be expressed

$$\sum_i P(1 \to i) = 1. \tag{17}$$

Note that the transition $1 \to 1$ is also permitted.

We have two conditions for reaching a steady state, namely *ergodicity* and *detailed balance*.

2.4.1 Ergodicity

The principle of ergodicity states that it is possible to reach any state 2 from any state 1 given a long enough Markov chain. This is an important constraint because every state i in the Boltzmann distribution P_i has a non-zero probability.

2.4.2 Detailed balance

The condition of detailed balance states that on average, the system makes the transition $1 \to 2$ as many times as $2 \to 1$. This can be expressed mathematically

$$P_1 P(1 \to) = P_2 P(2 \to 1). \tag{18}$$

Equation (18), implies that

$$\frac{P(1 \to 2)}{P(2 \to 1)} = \frac{P_2}{P_1} = e^{-\beta(E_2 - E_1)}. \tag{19}$$

2.5 Change in energy and magnetization by a spin-flip

Every time a spin is flipped, we need to compute the change in energy and magnetization of the system during the Markov chain. We exploit the fact that only one spin is flipped, all remaining spins keep their values fixed meaning $s_k^1 = s_k^2$. The energy difference between a state E_1 and a state E_2 with zero external magnetic field is then

$$\begin{aligned} \Delta E &= E_2 - E_1 \\ &= -J \sum_{<kl>} s_k^1 s_l^1 - J \sum_{kl} s_k^2 s_l^2 \\ &= -J \sum_{<kl>} s_k^2 (s_l^2 - s_l^1), \end{aligned} \tag{20}$$

where the sum runs over the nearest neighbours k of the spin. This term can be simplified by considering the values the flipped spin can take. If $s_l^1 = 1$, then $s_l^2 = -1$ and $s_l^1 - s_l^2 = 2$. Similarly, if $s_l^1 = -1$, $s_l^1 - s_l^2 = -2$. The change in energy can then be written

$$\Delta E = 2J s_l^1 \sum_{<k>} s_k. \tag{21}$$

By considering all possible configurations (table 3), we find that we only have five possible values for ΔE, $\Delta E = 8J, 4J, 0, -4J, -8J$.

We can compute the change in magnetization as well. Since only one spin at site k is flipped, the change is given by

$$\Delta M = M_2 - M_1 \tag{22}$$

$$= \sum_i s^1 - \sum_j s^2 \tag{23}$$

$$= s_k^1 - s_k^2 \tag{24}$$

$$= 2 s_k^1. \tag{25}$$

3 Method

3.1 Boundary conditions

When studying analytically solvable systems in statistical mechanics, we often let the systems approach the thermodynamic limit, that is, the number of particles approaches infinity. Numerically, we have to restrict our study to a finite $L \times L$ lattice size. The maximum system size we will use is 100×100. We use periodic boundary conditions to approximate a larger system. This ensures that our system will not have any boundaries as we are effectively projecting the two dimensional square lattice onto a sphere, as the upper row are in contact with the bottom row, and the same for the left and right side. Each spin now has four neighbours, and we are approximating the thermodynamic limit, as the boundaries play no role in the thermodynamic limit.

We can avoid if-tests and other time consuming operations to account for the periodic boundary conditions by introducing an index vector with the values $[L-1, 0, 1, 2, \ldots, L-2, L-1, 0]$. The value of the index-vector will be used as the spin-matrix-index.

3.2 The Metropolis Algorithm

The Markov chain Monte Carlo based Metropolis algorithm, which simulate the time-evolution of stochastic systems, is used to simulate the Ising model. The advantage of using the Metropolis algorithm, is that we avoid having to calculate the probability distribution function (PDF). Calculating the (PDF) requires heavy computations for every single possible state, which is numerically uneconomical. The Metropolis algorithm circumvents this problem because it only requires a function f proportional to the distribution density.

The following steps describes the Metropolis algorithm in a condensed way:

1. Initialize the system by an initial state which can be randomly generated. Compute the energy E_1 of this configuration.
2. Change the initial configuration by flipping the spin of an arbitrary site. Compute the energy of this new trial state E_2.
3. Compute the change in energy $\Delta E = E_2 - E_1$.
4. If $\Delta E \leq 0$, the new configuration is accepted. (The energy is lower than it was, and the system is progressing towards an energy minimum.)
5. If $\Delta E > 0$, compute $w = e^{-\beta \Delta E}$. If $w \geq r$, where r is a random number in the interval [0,1), accept the flipped state. Else the initial state is kept.
6. Update the expectation values.

These steps are repeated until a sufficiently good steady state is reached.

When the steps has selected L^2 random spins, we have completed a Monte Carlo cycle. The Monte Carlo part of the algorithm is the way we choose which spin to flip, and update the expectation values. The Metropolis part is the requirement for flipping a spin or not. Introducing more Monte Carlo cycles increases the precision of our results. For each Monte Carlo cycle the energy, energy squared, magnetization and magnetization squared, as well as the absolute value of the magnetization, are added to an array containing the sum of these values up until this state. After the algorithm is finished we calculate the expectation values for the quantities by dividing with the number of MC cycles.

This algorithm can be effectivized by pre-computing the possible energy changes, which are finite and shown to be $\Delta E = 8J, 4J, 0, -4J, -8J$ in section 2.5.

The algorithm determines whether a proposed move is implemented based on a transition probability and an acceptance probability. The advantage of the algorithm is that the transition probability can be unknown.

4 Results

4.1 The $L = 2$ case

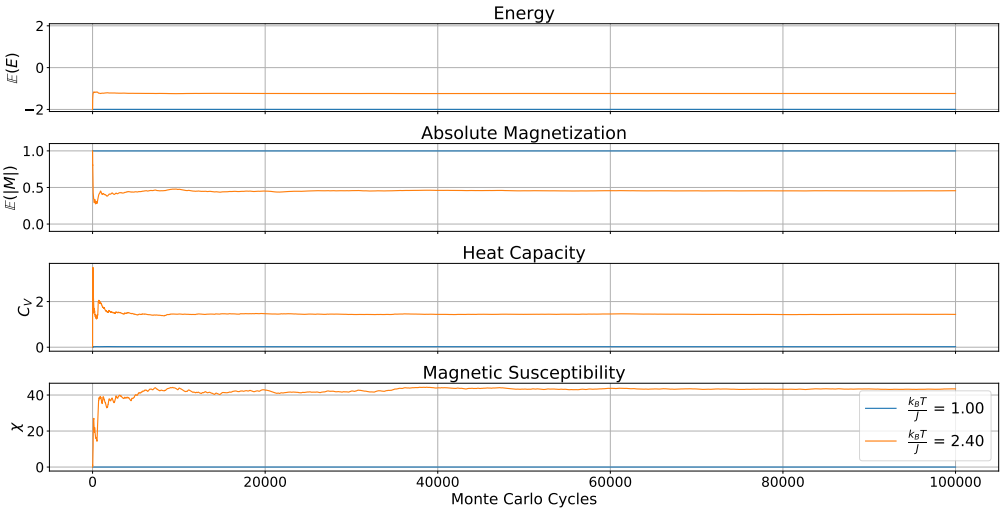
Table 1 shows a number of selected expectation values for the energy, specific heat capacity, mean absolute magnetization and magnetic susceptibility. From the table it is evident that the selected expectation values converges to the analytical values, and that it is necessary to have approximately 10^6 cycles to get the best estimates.

Table 1: Computed thermodynamic quantities for several Monte Carlo cycles per spin with $L = 2$ and $T = 1$ starting from an ordered spin configuration.

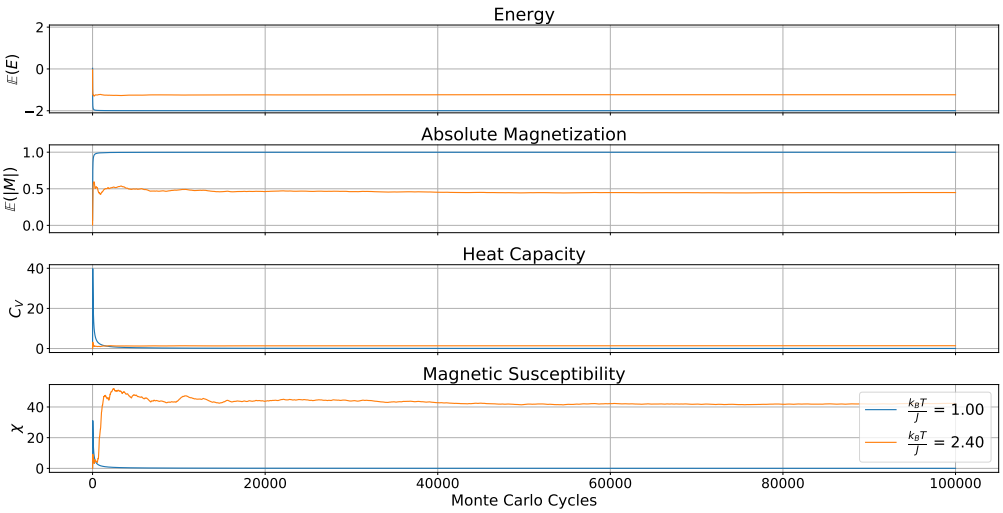
Cycles	$\langle E \rangle / L^2$	$\langle \lvert M \rvert \rangle / L^2$	C_v/L^2	χ/L^2
10^2	-1.8800	0.9650	0.9024	0.2379
10^3	-1.9880	0.9950	0.0954	0.0259
10^4	-1.9964	0.9987	0.0287	3.9656
10^5	-1.9957	0.9986	0.0346	3.9894
10^6	-1.9962	0.9987	0.0305	3.9910
Analytical	-1.9960	0.9987	0.0321	3.9933

4.2 Estimation of equilibration time

In figure 1 we plot the four thermodynamic expectation values of energy, absolute magnetization, heat capacity and magnetic susceptibility, as running expectation values over the number of MC cycles. They are plotted for the case of the initial state being the ground state where all spins point in the same direction, and secondly for a randomized initial spin state.



(a) Starting from the ground state.



(b) Starting from a randomized state.

Figure 1: Thermodynamic expectation values per spin as a function of Monte Carlo cycles. The system is a 20×20 lattice, for two temperatures $\frac{k_BT}{J} = \{1.0, 2.4\}$. The different thermodynamic quantities have slightly different equilibration times, but most notably is the temperature dependence. The system begins in the ground state with all spins pointing in the same direction.

4.3 Accepted spin-flips

To find the number of accepted spin configurations, we plot the number of accepted spin flips for select temperatures as a function of Monte Carlo cycles in figure 2. As explained in section 3.2, there will be more potential spin flips than Monte Carlo cycles.

We also studied the number of accepted spin-flips as a function of temperature, plotted in figure 3.

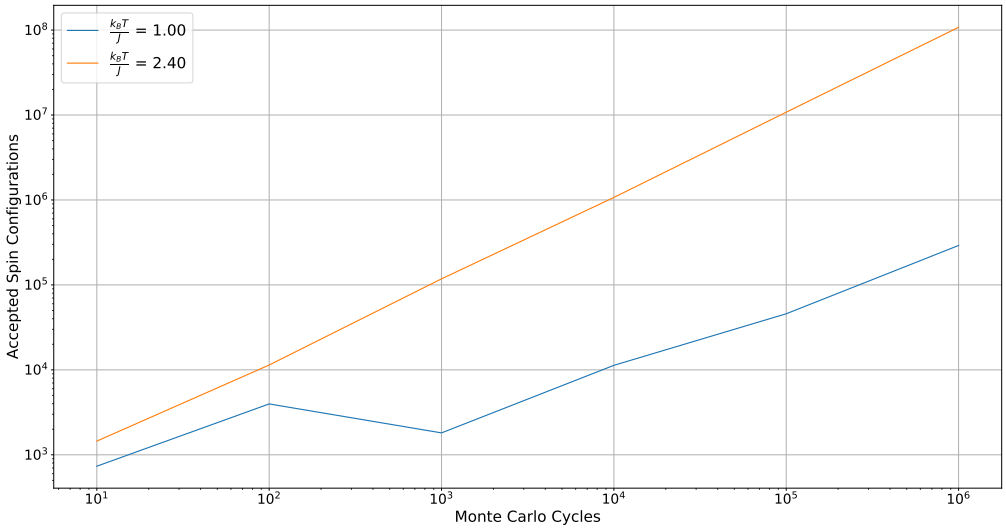


Figure 2: Number of accepted spin-flips as a function of Monte Carlo cycles. The system is a 20×20 lattice starting from a random configuration, and since each Monte Carlo cycle involves up to $20 \times 20 = 400$ spin flips, the number of spin flips tends to be higher than the number of cycles. We see a mostly linear relationship, while the lower temperature accepts fewer spin flips.

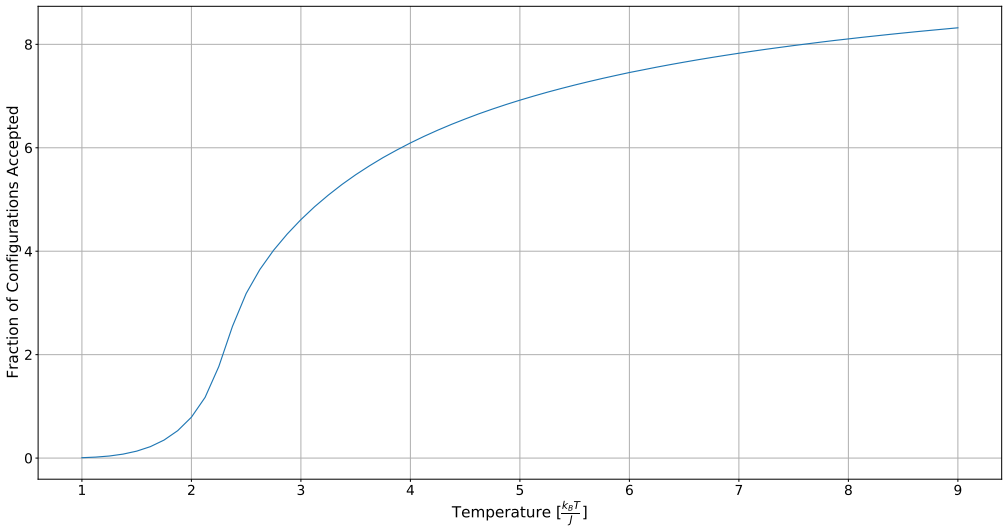


Figure 3: Fraction of accepted spin-flips as a function of temperature, for 10^6 MC cycles. The beginning state was randomized, and the resolution of the temperature is 0.125

4.4 Probability distribution function

We find the probability for the system to be in each state according to the simulation after equilibration time for select temperatures.

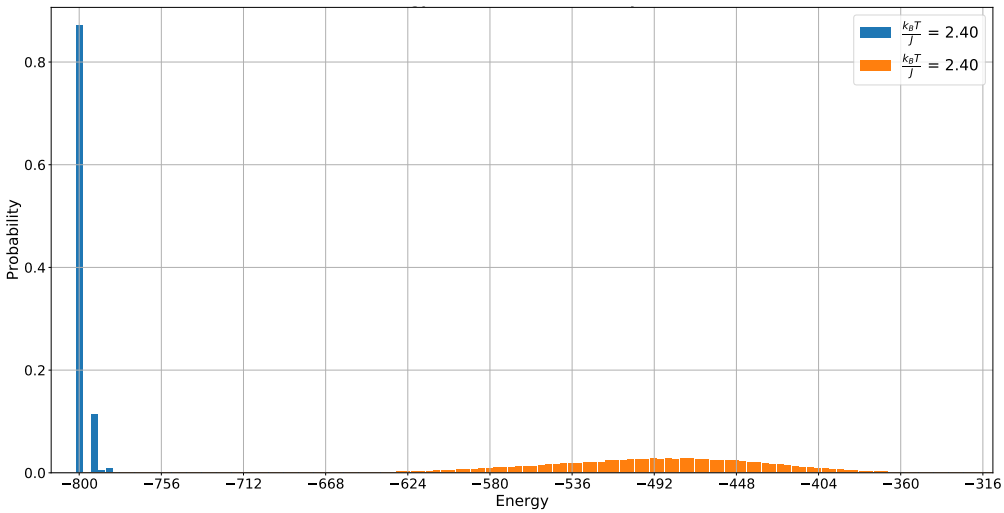


Figure 4: Distribution of states plotted against the energy of each state. The system is a 20×20 lattice, for two temperatures $\frac{k_BT}{J} = \{1.0, 2.4\}$. There is a clear difference between the two temperatures, with the $k_BT = 1.0$ case being in the ground state more than 80% of cycles, while the $k_BT = 2.4$ case being much more spread out around the $E = -492$ state. We have here used an equilibration time of 10% of the MC cycles, or 1000 cycles, such that only the data after this number of cycles has passed is included.

4.5 Phase transition and critical temperature

In figure 5 we plot the four thermodynamic values against temperature for four different lattice sizes, near the analytic critical temperature. This was done using parallellized code as the calculations are very time consuming.

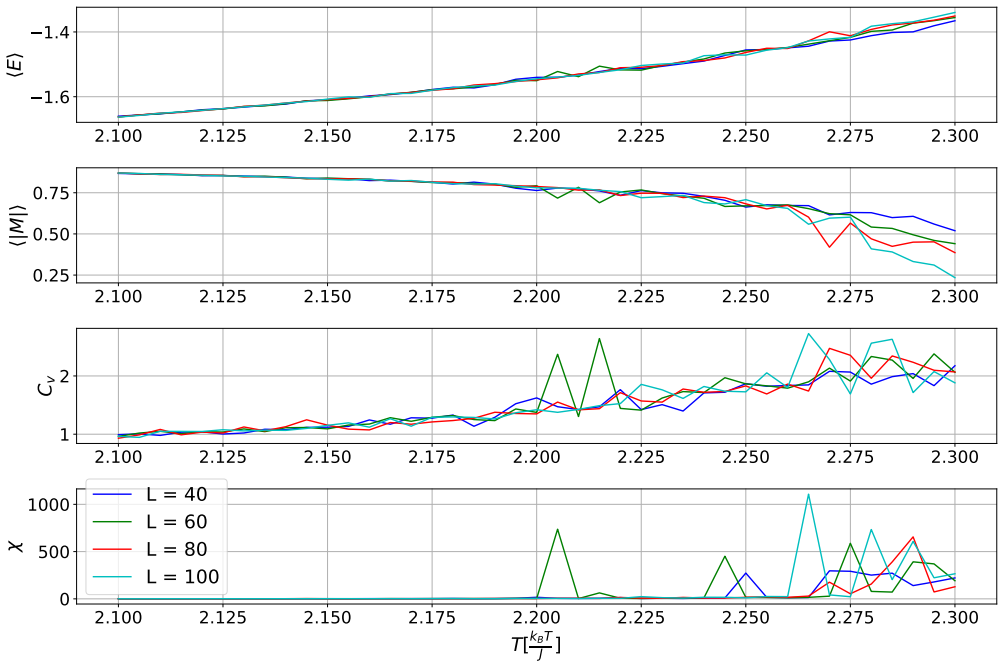


Figure 5: Behavior of the Ising model in two dimensions close to the critical temperature for different lattice sizes L. Comparison of the expectation values for energy $\langle E \rangle$ and the absolute magnetization $\langle |M| \rangle$, the specific heat C_v and the magnetic susceptibility χ for temperatures in the range $T \in [2.0, 2.3]$ with $\Delta T = 0.005$. There was done a total of 1E6 cycles per value of ΔT. All values are defined to be unit-less. Note that we have here cut off part of the plot to focus more on the interesting areas.

Table 2: Comparison of time elapsed in seconds before completion of simulation with and without running tasks in parallel. t is time taken without adding parallelization to our code and t_p is with.

L	t[s]	t_p[s]
40	3295	1624
60	7302	3534
80	12336	6071
100	19328	9213

In table [2] we compare the time taken to complete the simulations done in figure [5], but using $\Delta T = 0.01$ instead.

5 Discussion

5.1 Agreement with analytical results

From table 1, we observe that our code achieved a reasonable agreement with the analytical values for the $L = 2$ case with $T = 1.0$. The heat capacity is the least in agreement for the maximum 10^6 MC cycles, only conforming to the analytic value to one significant digit. The energy, magnetization and susceptibility all conform to at

least 3 significant digits. However, the accuracy with 10^5 MC cycles is not substantially worse, still agreeing to 3 significant digits fort everything but the heat capacity. Thus we calculate much of the subsequent values using 10^5 MC cycles for expediency, confirming their stability when plotting their evolution through MC cycles in section 4.2.

5.2 Estimation of equilibration time

The equilibration time is a measure of how many cycles it takes before the system reduces to its equilibrium state. Assessing this visually for figure 1, it appears that no more than 2×10^4 MC cycles are required for the energy, absolute magnetization and heat capacity to stabilize. However, the magnetic susceptibility is clearly still varying substantially up to about 1×10^5 MC cycles. However, this is only true for the case of $\frac{k_B T}{J} = 2.4$. When $\frac{k_B T}{J} = 1.0$, the ground state is reached very quickly, at just about 1×10^4 MC cycles all thermodynamic quantities have stabilized with a randomized start. For the case of beginning with the ground state, the equilibration time appears to approach 0 MC cycles, as all four quantities are stable during the entire simulation. We use a more conservative equilibration time of 10^4 MC cycles in further calculations. Longer equilibration times will also reduce the amount of data gathered, but further work could be in automatically verifying the equilibration time, perhaps individually for each thermodynamic quantity.

5.3 Accepted spin-flips

The number of potential spin flips scales as $L^2 \times N$, where N is the number of MC cycles. Thus we expect a linear graph when plotting the spin flips against MC cycles. In figure 2 we see that for $k_B T = 2.4$, this linear relationship is preserved. However, the lower temperature $k_B T = 1.0$ yields a graph that actually descends to fewer numbers of accepted spin-flips for 10^3 MC cycles. This can be explained by the fact that the low-energy system tends to be in the ground state, with all spins pointing in the same direction. The transition probability to the state directly above the ground state for $\frac{k_B T}{J} = 1.0$ is $\exp(-8) \approx 0.00034$, and so for small numbers of MC cycles, we expect some variation. The low temperature graph does seem to follow a roughly linear ascent otherwise.

It is important to note that the ground state and the state just above the ground state has an energy difference of $8J$, as explained in table 3. This is visible as a gap in the energy distribution in figure 4, between $E = -800$ and $E = -792$. Other states tend to have at least some spins that can be changed to yield an energy gap of $4J$, which means that the ground state is particularly unlikely to accept all spin changes.

In figure 3 we see the relationship between accepted states and temperature. The graph sharply rises near $\frac{k_B T}{J} = 2.25$, which happens to be the closest to the critical temperature that this resolution permits. It might be of interest as further work to create a graph like this but for larger lattices, to see if the same structure remains and whether it changes shape appreciably.

5.4 Probability distribution function

The distribution of states by energy is expected to follow a Maxwell-Boltzmann distribution, as we are using equation (1) to determine the probability of transition through the canonical ensemble. Figure 4 shows this, the higher temperature steady state produces a flattened, wider distribution of energies than the low temperature, almost ground state.

5.5 Finding the critical temperature

We want to solve eq (13) to find the critical temperature of the Ising model in two dimensions for a general lattice size L. To do so, we first need to find the constant a. As seen from (2.3), we need to find the approximate critical temperature of two finite lattices and then make an estimate of a, using $\nu = 1$. Since we have done simulations over four finite lattice sizes, we will find an average value of a by calculating over all possible combinations of lattices, but first we need to determine where the critical temperature is for the different lattices. We know that the theoretical critical temperature $T_C(L = \infty) \approx 2.269$ as given by Lars Onsager [7], and we can see in our plots of the different sized L's in [5] that in the $T \in [2.250, 2.30]$ range something happens with our model. If we focus in on the plot over the specific heat C_v, we can read of the values of T that maximize C_v. We use C_v because we know that as the system approaches the critical temperature, the heat capacity increases as $T \to T_C \to C_v \to \infty$. It is also clear that the values of C_v are slightly more stable than e.g the susceptibility χ, which means that the results we find will be less prone to numerical errors and instabilities.

When we now calculate the value of a, we find that $a = -0.6277\ldots \approx -\frac{2}{3}$. Inserting this value into eq (13) for each L and then calculating the average gives us the critical temperature $T_C(L = \infty) \approx 2.273$. This gives us a difference of $4 \cdot 10^{-3}$ and a percent error of $\delta = 0.17\%$ compared to the analytical solution. This is quite a good result, but could most likely be improved by simply running simulations of even more lattices and and even higher resolution. It is also quite clear that some computation time was wasted in the range of temperatures near $T = 2.0$. As there is nothing of particular value to be found here, at least for the case of finding the critical temperature, it would prove more efficient to narrow the range of T to something like $T \in [2.20, 2.30]$ and then increase the resolution to $\Delta T \leq 0.001$. Finally, it would increase our accuracy to run each temperature over more cycles than 1E6, however as the cycles increase the returns are diminishing compared to the compute time required.

5.6 Parallelization

Simulating the Ising model for two dimensions is quite a slow process if done on only one CPU core. It is therefore of great interest to share some of the burden from one core to several. We see from 2 that when our code runs on several cores that the speed of our code increases by approximately a factor of 2. This is not really unexpected as one would assume that many cores would be better than one, and that is in fact what we have observed. We implemented parallelization using the OpenMPI library, running on four physical cores. It does not seem like OpenMPI supports Hyperthreading/non - physical cores without some extra tinkering on our part so there might have been more performance to gain, although using non-physical cores could also be less efficient given the tasks we were running.

6 Conclusion

After having made Monte Carlo simulations of the 2-dimensional Ising model for the lattices, we have found results that fit quite well with the analytic results. The 2×2 lattice was found to have an agreement of 4 significant digits on expected energy and absolute magnetization, 3 significant digits on magnetic susceptibility, and 1 significant digit on heat capacity, all with 10^6 Monte Carlo cycles. The equilibration time for the 20×20 lattice seemed to be about 1000 MC cycles, and we also found the probability distribution of state to conform with the expected Maxwell-Boltzmann distribution.

The critical temperature we found for a lattice of infinite size was $T_C(L = \infty) = 2.273$ which had just an error of $\delta = 0.17\%$ compared with the known analytical solution, and we discovered that the use of parallel computing techniques could improve the execution time of our program by about a factor of 2.

Future work could involve further optimization of code, like further optimizing the parallelization even more by splitting the work across all cores in a more efficient way, as well as finding ways to automatically determine the equilibration time.

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A Appendix

A.1 Source code

Github repository with codes and figures can be found at `https://github.com/idadue/ComputationalPhysics/tree/master/project4`.

A.2 Possible changes of energy

Table 3: The five different possible changes in energy, ΔE in a two dimensional lattice, when only interacting with the nearest neighbours.

Initial state	Flipped state	Initial E	Flipped E	ΔE
$\begin{array}{ccc} & \uparrow & \\ \uparrow & \uparrow & \uparrow \\ & \uparrow & \end{array}$	$\begin{array}{ccc} & \uparrow & \\ \uparrow & \downarrow & \uparrow \\ & \uparrow & \end{array}$	-4J	4J	8J
$\begin{array}{ccc} & \downarrow & \\ \uparrow & \uparrow & \uparrow \\ & \uparrow & \end{array}$	$\begin{array}{ccc} & \downarrow & \\ \uparrow & \downarrow & \uparrow \\ & \uparrow & \end{array}$	-2J	2J	4J
$\begin{array}{ccc} & \downarrow & \\ \downarrow & \uparrow & \uparrow \\ & \uparrow & \end{array}$	$\begin{array}{ccc} & \downarrow & \\ \downarrow & \downarrow & \uparrow \\ & \uparrow & \end{array}$	0	0	0
$\begin{array}{ccc} & \downarrow & \\ \downarrow & \uparrow & \downarrow \\ & \uparrow & \end{array}$	$\begin{array}{ccc} & \downarrow & \\ \downarrow & \downarrow & \downarrow \\ & \uparrow & \end{array}$	2J	-2J	-4J
$\begin{array}{ccc} & \downarrow & \\ \downarrow & \uparrow & \downarrow \\ & \downarrow & \end{array}$	$\begin{array}{ccc} & \downarrow & \\ \downarrow & \downarrow & \downarrow \\ & \downarrow & \end{array}$	4J	-4J	-8J

A.3 Analytical expressions for a simple 2×2 lattice

Consider a 2×2 lattice, each lattice point with spin ± 1, this model has $s = 2^4 = 16$ different configurations as shown in table 4. With the size of this model, it is possible to calculate analytically the expectation values with the partition function, as it only contains 16 elements (most of which are zero).

The partition function for the 2×2 lattice is given by

$$Z = \sum_i e^{-E_i \beta} = 12 + 2e^{8\beta} + 2e^{-8\beta} = 4(3 + \cosh 8\beta),$$

where $\beta = 1/k_B T$.

The expected energy is then

$$\langle E \rangle = -\frac{\partial}{\partial \beta} \ln Z = -\frac{\partial}{\partial \beta} \ln(4\cosh(\beta 8J) + 12) = -8J \frac{\sinh(8\beta J)}{\cosh(8\beta J) + 3},$$

Table 4: All configurations of a 2×2 Ising model. The table displays the degeneracy, energy and magnetization where $N_\uparrow$ is the number of spins up.

$N_\uparrow$	$\Omega(E_i)$	E_i	M_i
4	1	$-8\,\mathrm{J}$	4
3	4	0	2
2	4	0	0
2	2	$8\,\mathrm{J}$	0
1	4	0	-2
0	1	$-8\,\mathrm{J}$	-4

and the variance of the mean energy is

$$\begin{aligned}\sigma_E^2 &= \langle E^2\rangle - \langle E\rangle^2 \\ &= \frac{1}{2e^{-\beta 8J} + 2e^{\beta 8J} + 12}(2\cdot(-8J)^2\cdot e^{\beta 8J} + 2\cdot(8J)^2\cdot e^{-\beta 8J}) - \left(-8j\frac{\sinh(8\beta J)}{\cosh(8\beta J)+3}\right)^2 \\ &= 64J^2\left(\frac{\cosh(8\beta J)}{\cosh(8\beta J)+3} - \left(\frac{\sinh(8\beta J)}{\cosh(8\beta J)+3}\right)^2\right).\end{aligned}$$

We can now simply insert the variance of the mean energy to get the expression for the specific heat capacity

$$\begin{aligned}C_V &= \frac{\sigma_E^2}{k_B T^2} \\ &= \frac{1}{k_B T^2} 64J^2\left(\frac{\cosh(8\beta J)}{\cosh(8\beta J)+3} - \left(\frac{\sinh(8\beta J)}{\cosh(8\beta J)+3}\right)^2\right).\end{aligned}$$

The mean magnetisation is found by adding all possible states and dividing by the partition function

$$\langle M\rangle = \frac{1}{Z}\sum_i M_i e^{-\beta E_i} = \frac{1}{Z}(-4e^{8\beta J} - 8e^0 + 8e^0 + 4e^{8\beta J}) = 0.$$

The expected absolute magnetisation is non-zero and given by

$$\langle |M|\rangle = \frac{1}{Z}\sum_i |M_i| e^{-\beta E_i} = \frac{1}{Z}(4e^{8\beta J} + 8e^0 + 8e^0 + 4e^{8\beta J}) = \frac{4 + 2e^{8\beta J}}{\cosh(8\beta J)+3}.$$

We calculate the variance of the mean magnetization, needed for the calculation of the magnetic susceptibility

$$\begin{aligned}\sigma_M^2 &= \langle M^2\rangle - \langle M\rangle^2 \\ &= \frac{32}{Z}(e^{8\beta J}+1) - 0 \\ &= \frac{8(e^{8\beta J}+1)}{\cosh(8\beta J)+3}.\end{aligned}$$

The magnetic susceptibility is then

$$\begin{aligned}\chi &= \frac{1}{k_B T}\sigma_M^2 \\ &= \frac{1}{k_B T}\frac{8(e^{8\beta J}+1)}{\cosh(8\beta J)+3}.\end{aligned}$$