1 Introduction

This computational project centers on using numerical techniques to simulate a 2D Ising model. In particular we use the Metropolis-Hastings algorithm to test if a flip of any individual spin should occur. This occurs by considering the resulting change in the Hamiltonian defined as

$$H = -J \sum_{,j\rangle} \sigma_i \sigma_j - \mu B \sum_i \sigma_i,$$

where we set $J, \mu, k_B = 1$. We use periodic boundary conditions, i.e. our Ising model exists on a torus so the all 4 sides of a square grid wrap around. If our Ising model is infinitely large, there is a critical temperature at $T_c = 2.27$ which results in a phase transition.

To consider if we should accept any individual flip we consider the change in energy ΔE that would occur as a result of the flip. If $\Delta E < 0$ we accept the flip as it pushes the state to a lower energy state. If instead $\Delta E > 0$, we accept the flip with probability $e^{-\frac{\Delta E}{k_B T}}$. This is the Metropolis Algorithm.

We aim to do 3 tasks in this report, firstly, consider the time it takes for the model to reach equilibrium, secondly, simulate an Ising model under different conditions and compare to various theoretical results and thirdly, test parallelisation using OpenMP.

We use various theoretical results presented in the task sheet, namely the absolute magnetisation per spin,

$$|M| = \begin{cases} \left[1 - \sinh^{-4}\left(\frac{2J}{k_B T}\right)\right]^{1/8}, & T < T_c. \\ 0, & T > T_c. \end{cases}$$

the specific heat per spin

$$c = \frac{\mathrm{var}(E) N_s}{k_B T^2},$$

and the magnetic susceptability per spin

$$\chi = \frac{\mathrm{var}(|M|) N_s}{k_B T}.$$

2 B1: Markov Chain Monte Carlo

Here we implement the basic Metropolis algorithm to simulate the Ising model. We begin by defining functions to initialise a lattice which we use $vector < vector < int >>$ to store (up is 1 and down is -1). To ensure we do not have a local minimum, we initialise with an 85% bias towards spin up. We also define a function to print the lattice which just goes through each row and column and prints the entry as either $\uparrow$ or $\downarrow$.

To compute the initial energy we sum over the pairs of spins and add together each spins neighbours (with wrap around boundary conditions), multiply by the spin and subtract from a running total. We then half the result as we counted each interaction twice. To find the initial magnetisation we just take the sum of all spins.

With this we can define a function to calculate the change in energy which calculates the sum of neighbours for a proposed spin flip and twice the multiplication of these. We can also add in a contribution if B is non-zero of $2\sigma_i B$ to make it easier later on.

With this we can run a simulation for 2000 sweeps and for 16x16 spins where we choose a random site at each instance to test if we should flip rather than going in order from first to

last. This is for 3 reasons. Firstly it avoids systematic bias: if we update spins in a fixed order (e.g., sweeping row by row), we introduce correlations that may affect equilibrium properties. Secondly, more realistic thermalization: real physical systems undergo stochastic thermal fluctuations, and random updates better mimic this behavior. Thirdly, prevents artificial artifacts: orderly updates can create artificial patterns, especially at low temperatures where domains form.

We then take the output every sweep and save it to a txt file for plotting and analysis, which is done in python. We finally print the lattice to test if the algorithm appears reasonable.

When plotting we use python's inbuilt features to track the cumulative mean and plot on a log x-axis to yield figure 1. This allows us to see that after 10^3 sweeps, the cumulative mean is quite stable and hence suggests that a burn in time of 1000 sweeps and an averaging time of 1000 sweeps will yield reasonable results. We use this to inform our analysis on thermodynamic properties.

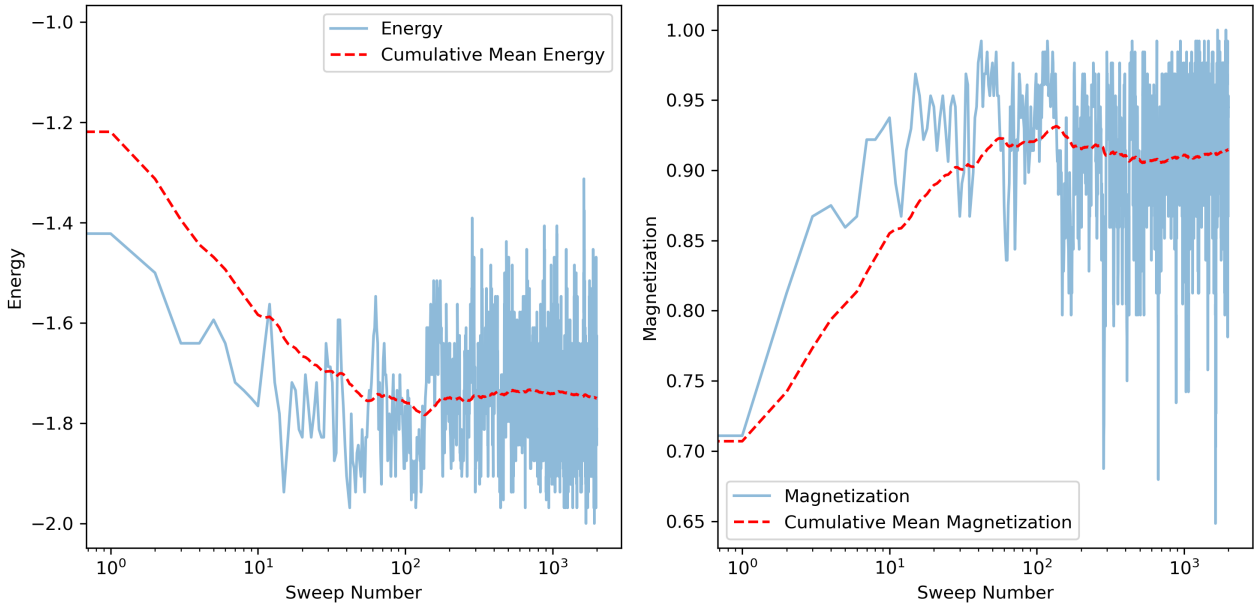

Figure 1: Energy and Magnetisation per spin as a function of sweep number with cumulative mean for $T = 2$ and log x-axis. This plot shows how the initial energy and magnetisation is quite distinct from the final state and suggests that a burn in time of 800-1000 sweeps is reasonable for temperatures close to T_c.

3 B2: Thermodynamic Properties

3.1 Relationship with Lattice Size

To analyse the thermodynamic properties we can consider how the quantities of energy per spin, magnetisation per spin, susceptibility per spin and specific heat per spin as functions of temperature change for different lattice sizes. Note that we chose to use the per spin version of these quantities as if not, the results would be difficult to interpret due to changing lattice size. We choose to use lattice sizes of 8,16,32 and 64 (side lengths) with temperatures equally spaced between 0.3 and 5. We run the simulation looping through these conditions and use the final state of 1 temperature as the initial state of the next, we give the simulations 1000 sweeps of burn in time and 1000 sweeps to record the relevant quantities and then save data in a txt file to then plot using python.

We show our results in figures 2 and 3 where we use standard error for the error bars. From the first plot we can see that around the critical temperature a clear phase transition occurs where the magnetisation goes from 1 to near 0 almost instantly, and importantly the drop is sharper as the lattice we consider gets larger. We also see that for all 4 sizes the energy plot remains fairly smooth but the smoothest is clearly for $L = 64$.

From the specific heat and magnetic susceptability plots we can see that that a clear spike in both quantities are around the critical temperature which suggests that the numerical simulation can be accurately used to find theoretical quantities. Importantly, it appears that as the lattice size gets larger, the quantities of interest get more accurate. This aligns with theory where the critical temperature is calculated in the thermodynamic limit of $L \to \infty$. As such, this shows that our simulation is accurate and useful in the calculation and comparison of relevant theoretical properties.

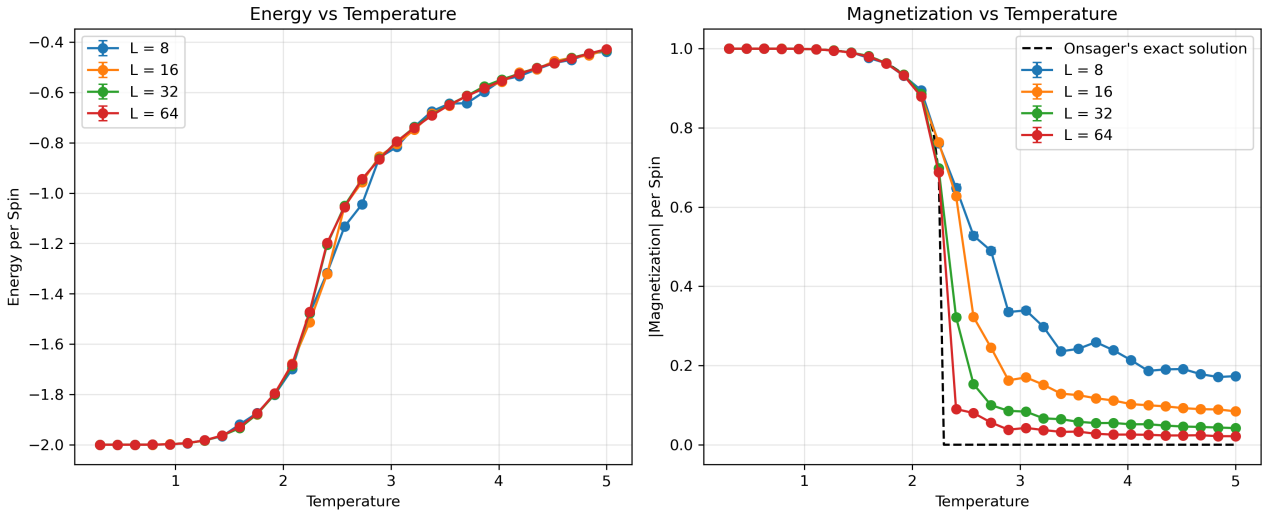

Figure 2: Plot of energy per spin and magnetisation per spin vs temperature for 4 different lattice sizes. We can clearly see that all 4 lattices for energy per spin follow the same relationship but the larger the lattice the less potential noise exists. For Magnetisation we can clearly see the larger the lattice, the closer to theoretical results we get.

3.2 Influence of Applied Magnetic Field Strength

To test the effect of an applied magnetic field on the Ising model we can plot the same quantities for $L = 16$ and a variety of different values for B. We will consider the same spread of temperature values and the same burn in time. Importantly, the application of a magnetic field gives the lattice a preferred direction by weighting up or down as a negative contribution to the energy. This means our calculation for change in energy can consider this and thus change the dynamics of the system. Because we only consider the absolute magnetisation we can consider 6 values for B between 0 and 0.5 inclusive.

We show our results in figures 4 and 5 where we can see that the application of a positive magnetic field has the effect of shifting the curves to the right for both energy and magnetisation. This is reasonable as we are effectively increasing the critical temperature needed to push the Ising model out of the ordered state as there is an external factor which 'rewards' order. For specific heat and susceptability we see that the magnetic field pushes the curve right again suggesting that the effective critical temperature is increased. It also reduces the peak height which is because the variation in the magnetism is decreased due to a preferred direction of the spins.

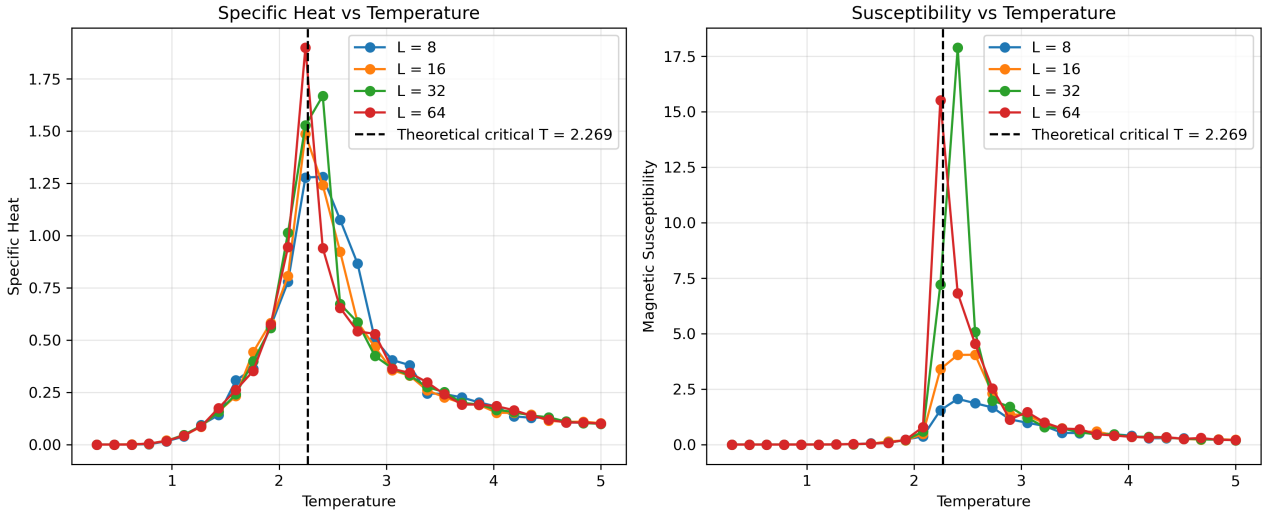

Figure 3: Specific heat and magnetic susceptability per spin showing a clear spike around the theoretical critical temperature and closer agreement for larger lattice sizes.

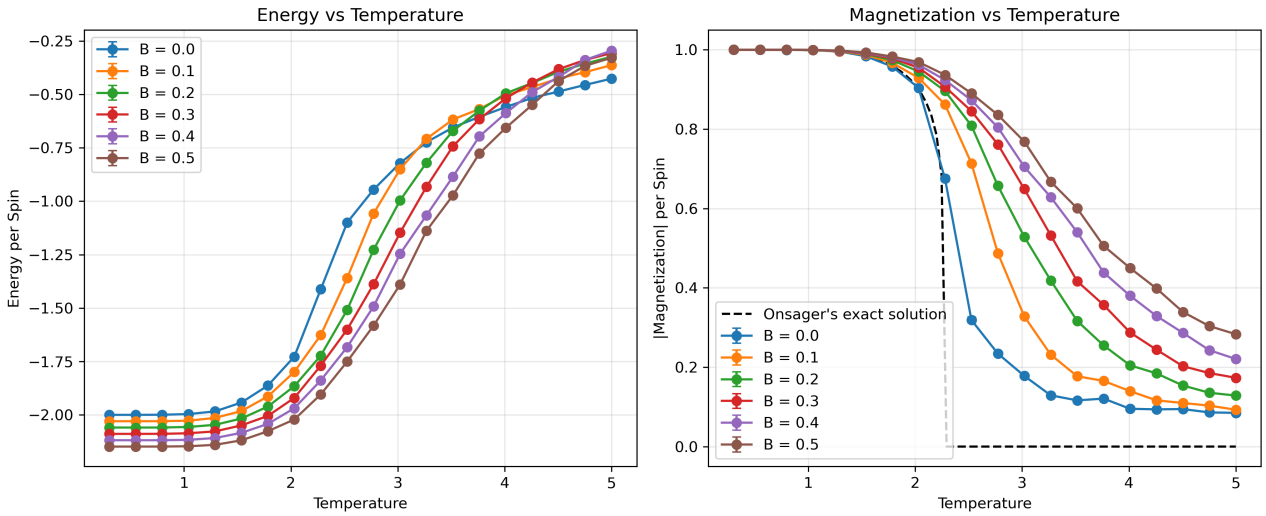

Figure 4: Energy and magnetisation per spin against temperature for different B values, we see that application of a magnetic field shifts the curve right indicating a higher effective critical temperature.

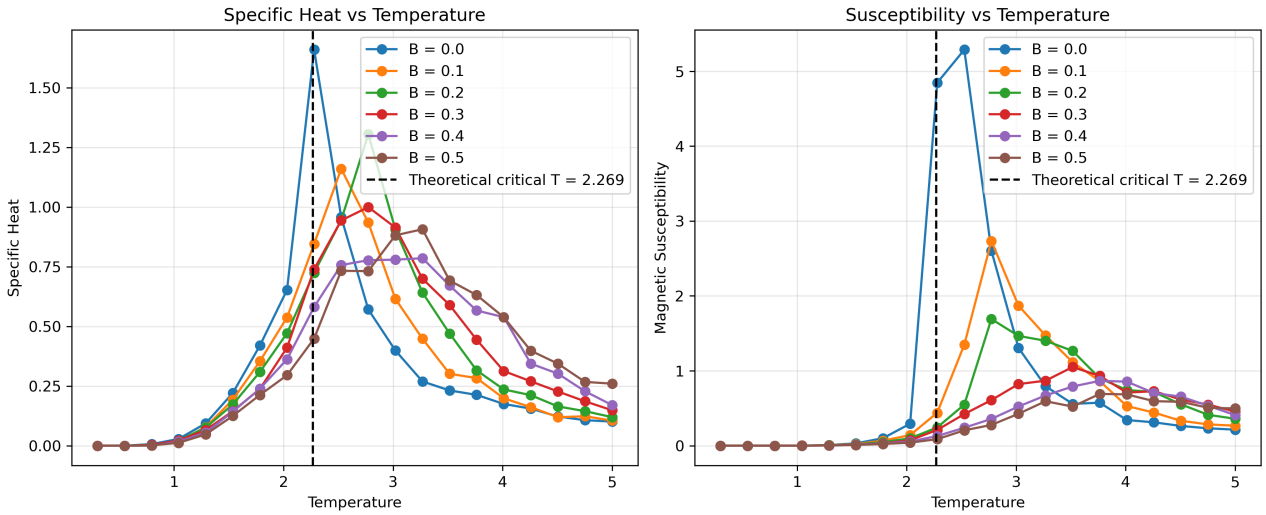

Figure 5: Specific heat and susceptibility vs temperature for different B values. Again we see the same trend of curve shifted to the right.

3.3 Power Law Scaling

Our next task is to consider the power law scaling of magnetisation and magnetic susceptability. We wish to test if we can reproduce the power scaling laws

$$|M| \sim |T - T_c|^{\beta}, \quad \chi \sim |T - T_c|^{-\gamma},$$

where $\gamma = 7/4$ and $\beta = 1/8$ in 2 dimensions. We run the simulation for $L = 256$ with 100 temperatures between 2 and T_c and $B = 0$ and save the output data in a txt file for analysis. To yield accurate results we run the simulation for 2000 sweeps and only save the last 1000 as we are very close to the critical temperature.

To analyse and plot the data we calculate the absolute magnetisation and susceptibility and plot against $|T - T_c|$ on a log-log plot. We can then yield the plots shown in 6. Note that a large amount of experimentation was conducted to get these plots appearing with an appropriate fit as I tested changing the number of temperatures, the lattice size, the number of sweeps and the range of temperatures. For the magnetisation data, we plot for temperatures less than 2.25 as any data closer to T_c reduces the accuracy of our fit quite a bit. Similarly, for susceptability, we only plot temperatures up to 2.2. We chose a large lattice size as the power laws only appear viable when we are the thermodynamic limit of $L \to \infty$. As such, when experimenting, the power laws were not showing up unless we had $L \geq 256$.

Now we can consider the physical relevance of these plots. The core reason why we see these power law scaling relations is because of the assumptions we are making. Our model is simultaneously competing between energy minimisation and entropy maximisation, and below T_c we see the spontaneous symmetry breaking where we go from an unordered state to an ordered state. Right below T_c we are hence expecting an ordered state but because of the spurious correlations from our periodic boundary conditions we do not see this occur in the simulations. This means instead of an instantaneous drop as we would expect for $L \to \infty$, we get a power law scaling relationship for magnetisation and hence susceptibility as well. In particular, the susceptability quickly approaches infinity by the power law scaling because it measures how sensitive the system is to small external field. Hence, because just below the critical temperature, the correlation length diverges - as we expect a fully ordered model and so every spin is correlated with every other spin - it means that any tiny change to an

external magnetic field will cause the model to flip to that direction. As such, we expect the susceptibility to diverge to ∞ at T_c from below. As the temperature gets a bit lower than T_c, there is less sensitivity to a magnetic field as the temperature is low enough that the model will fall into an ordered state based more on its initial condition than by a small external field. As such, these plots are representative of the assumptions we make in the computational Ising model where the periodic boundaries cause spurious correlations around the edges of the lattice and increase the correlation length artificially.

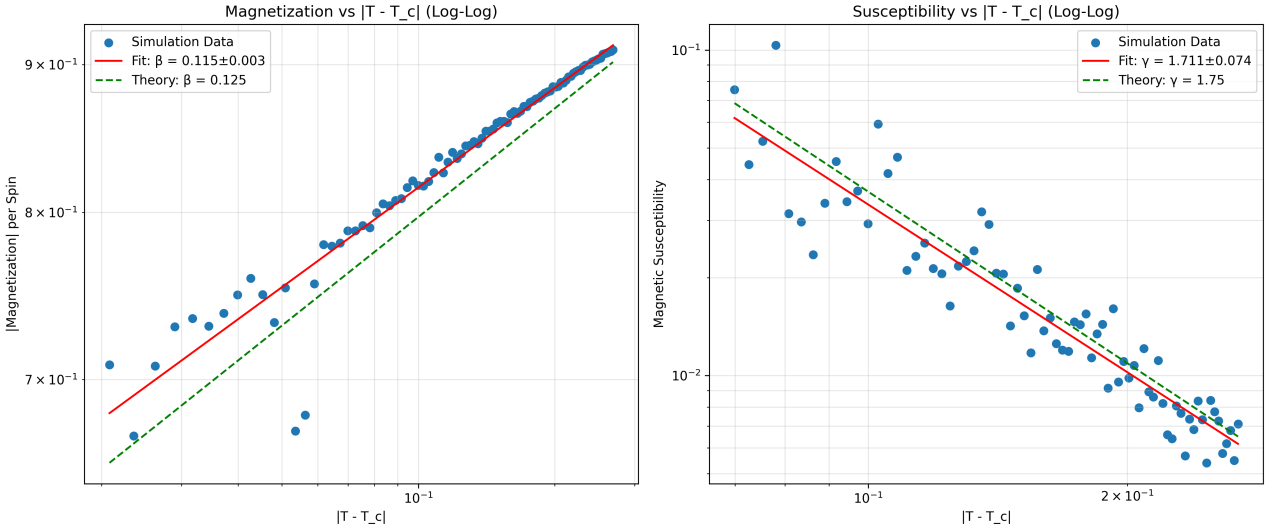

Figure 6: Plot of the finite size power scaling laws of the Ising model for both magnetisation and susceptibility. We see that both relations follow a linear relationship on a log log plot with approximately the correct gradient. We note however that we can yield a better fit by vertically shifting the theoretical relationship. Additionally, we should note that the range of temperatures plotted were chosen for the closest fit and the lattice size and number of sweeps were as well. In all, this plot shows the power law scaling which demonstrates the changing correlation length around the critical temperature which causes spontaneous symmetry breaking and shows us that spurious correlations across boundary conditions can produce artifacts compared to theory.

4 B3: OpenMP implementation

As the Ising model is a simulation, it is natural to consider if there are ways to speed up the process of testing flips. One method is to use multithreading whereby a for loop is run using multiple CPUS to do a task that is independent of other CPUS.

The Ising model can be slightly modified to do exactly this where instead of testing random flips, we test the even and odd rows separately, this is to ensure that we never test neighbouring spins on different threads at the same time (i.e. a race condition). Once we have modified the code to do this, we can wait for all threads to come together after a sweep and then print the outputs, we can then continue to do this for all the sweeps. Note that we choose to set $L = 128$ as the potential advantages of multi threading are more pronounced at larger lattice sizes.

We can test the results from the multithreading and see that we clearly get the same results as in earlier parts of the question with the smooth curves and sharp change around the critical temperature (fig. 7). We see this is true independent of the number of threads we are using which verifies that we are at least simulating the correct properties of the Ising model.

Using these simulations we can also test how long the Ising model takes to simulate for different number of threads. This is done by timing how long it takes to do the loops over all temperatures. Note that the assignment only asks us to do it for a fixed temperature but in order to test its usefulness in real applications for Ising Model simulations I think it is more valid to test the effect of parallelisation over a number of temperatures as well. In addition, this simplifies the total amount of code and the output as I only have to run the parallelisation cpp file once rather than doing it again for a fixed temperature or only saving time lengths for a fixed temperature. The results of this analysis is shown in figure 8. We can clearly see a non-linear speedup using parallelisation with the lowest time happening at 4 threads and an increase in time happening after 4 threads. This is likely because my computer has 4 physical cores. While my computer has 8 logical cores, when the software is using more than the number of physical cores, it needs more time to initialise and can spend a substantial amount of time setting up for parallelisation. Additionally, the logical cores are not always as efficient as the physical cores.

I also have 2 other theories for why we observe this non-linear behaviour. Firstly, if each thread has little work to do, the overhead of creating and managing threads might outweigh the performance gains which suggests that using a larger grid would potentially yield better speedups. Secondly, the critical barrier and master sections make the time scaling worse for more threads as when you have more threads there will be more waiting time where threads are not simulating or testing sweeps (i.e. wasted time).

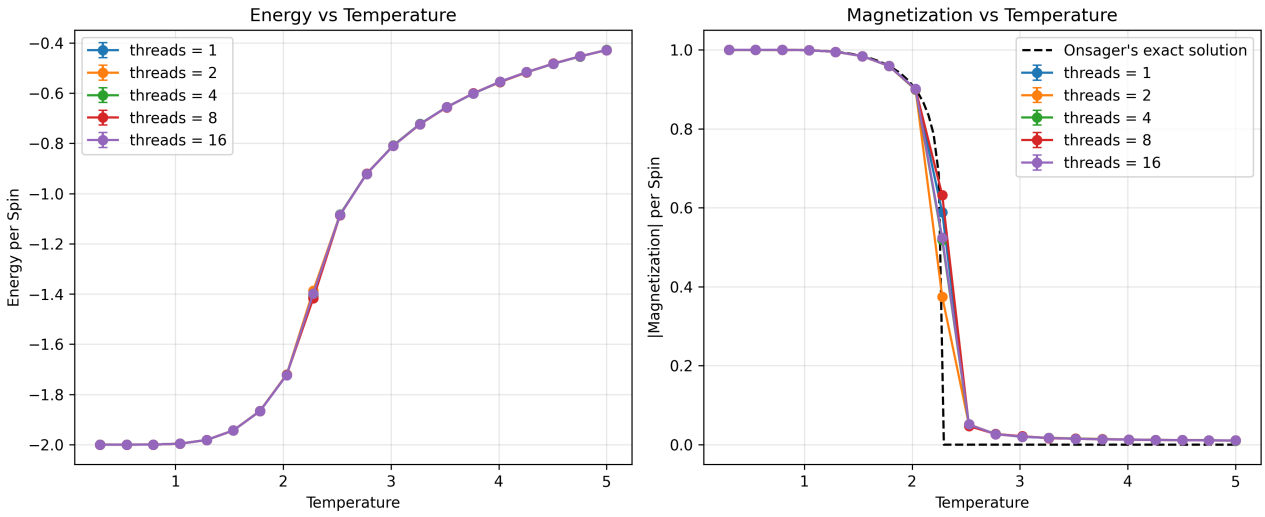

Figure 7: Plot of the energy and magnetisation per spin of the Ising model for a range of temperatures under different number of threads using OpenMP parallelisation. We see the same trends are reproduced independently of the number of threads suggesting that the application of Multithreading still yields reasonable results for the Ising model simulation and does not change the thermodynamic properties.

5 Conclusion

In this computational project we explored the 2D Ising model via markov chain monte carlo simulations using the Metropolis algorithm. We investigated a number of interesting phenomenon beginning with burn in time required for the model to achieve equilibrium and average time to take reasonable data. We then used this to explore how properties which depend on T, change

Figure 8: Plot of the simulation time against the number of threads where we see a non-linear speedup for 1-4 threads and then an increase in time after 4 threads.

with lattice size as we increase the number of spins and get closer to approximating the thermodynamic limit $L \to \infty$. We found clear signs that increased lattice size aligned with increase in accuracy to theoretical results and smoother curves with less noise. We also used this to show the numerical critical temperature is very close to the theoretical critical temperature.

When investigating the effect of an applied magnetic field we saw that curves for absolute magnetisation and energy are shifted to the right, suggesting an increase in the effective critical temperature and less sharp phase transitions. This logically follows as the magnetic field biases the grid towards a certain orientation and prefers a more ordered system, thus requiring more randomness to move away from the ferromagnet regime.

We explored the power law scaling of magnetisation and magnetic susceptibility to show alignment with theory and to represent that physically in the system we see an asymptotic increase in correlation length at the critical temperature which results in non-analyticity for magnetisation and susceptability at the critical temperature.

Finally, we used OpenMP to see if multithreading is useful and applicable in the 2D Ising model situation. We see that independently of the number of threads, the simulation appears to work correctly and reproduce results shown previously, this suggests multi-threading can be used and is not likely to cause errors in the simulation. We then showed that the time taken for the implementation using 4 threads was non linearly reduced from 1 thread suggesting that the implementation is not only accurate but also useful if we wish to complete large scale simulations.

Overall, this report presented an in depth exploration of the 2D Ising model via simulations and was useful to explore thermodynamic properties and interesting behaviour of the model under varying conditions. All code is available on Github.