Computational Treatment of the Ising Model using Metropolis Monte Carlo Methods

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Abstract

The early 20th century saw the introduction of the eponymous Ising model by Ernst Ising and Wilheim Lenz, a novel yet simple theory for the explanation of ferromagnetic behaviour. Modern computational models of the Ising model are combined with Monte Carlo methods, which simulate the change of spin states within the system. Together, these allow for ferromagnetic systems to be studied in even greater depth, allowing for control over specific boundary conditions. This consideration involved a variant of the Ising model restricted to binary-valued spin states. Using this simplified model, the magnetisation of the system was investigated as a function of the applied temperature to observe latent trends. Estimates for the equilibrium averages of both energy and magnetism were further determined, and the results compared to mean-field theory and the exact Onsanger solution for the model.

1. Introduction

During the mid-20th century, phase transitions experienced a marked popularity within the physics community at the time, with the 1940s and 1950s being a period of intense research. This was most apparent within the field of statistical mechanics, with phase transitions being a property characterising many statistical systems [1]. Of particular interest was the phase transition exhibited by ferromagnetic materials at the Curie temperature, T_c, of the material. It had been observed that at T_c, ferromagnets would undergo a phase transition to become a paramagnet, losing the long-range ordering of its spins.

The Lenz-Ising model, as it was originally named, was proposed in 1920 by then-student Ernst Ising and his supervisor, Wilheim Lenz [2]. Ising had been studying behaviour of ferromagnets, and Lenz and Ising put forward their model as an improved theoretical representation for the behaviour of ferromagnets and paramagnets on the microscopic level, based on experimental observations.

2. Theory and method

2.1 The Ising Model

In 2 dimensions, the Ising Model provides a simple model of the phase transition between the low-temperature, ordered state of a system of spins and the high-temperature, disordered state [3].

For a system with spins $s_i = \pm 1$, corresponding to spin 'up' or spin 'down' states respectively, let there be N sites on a square lattice. Each site will be then assigned a spin, which can be in either state. For the i-th spin, its energy is given by

$$E_i = -h_i\, s_i \tag{1}$$

with

$$h_i = \sum_{j \text{ n.n. of } i} (J s_j) \tag{2}$$

J denotes a positive number describing the interaction strength between each spin; n.n. is shorthand for the "nearest neighbour" spins; j refers to a site that is different from i, with s_j the spin at the j-th site. The quantity h_i can be regarded as the local magnetic field for a particular spin i. When aligned with magnetic fields, the spins are expected to have a low energy [4].

The total energy of the system given by the Ising Model is then the sum over the energies of all spins i. From the definition of individual spin energies in equation 1:

$$E = \frac{1}{2}\sum_i E_i \tag{3}$$

Combining this definition with the result of equation 2 then gives an expression for the energy, as a sum over all pairs of nearest neighbour spins:

$$E = \sum_{\langle ij \rangle} (-J s_i s_j) \tag{4}$$

Here, the summation notation over $\langle ij \rangle$ is convention for a sum over all nearest neighbour pairs, rather than denoting an expectation value.

In physical terms, the Ising model can be considered in terms of electron spin orientations, s_i. While a real magnet may have its electron spins aligned to other directions than simply up or down, allowing s_i to take a wider range of values, certain materials have been found to manifest binary spins. At the same time, restricting $s_i = \pm 1$ allows for a simpler model and analysis. However, as with any simplified model, it will be expected that the simulation may differ from experimental results [4].

As the Ising model deals with ferromagnetism, particular quantities to consider are the magnetisation per spin

$$M = \frac{1}{N}\sum_i s_i \tag{5}$$

and the energy per spin, *E/N*. As s_i can only take two values, for a large value of *N*, if the majority of spins are 'spin-up', M ≈ 1; and the opposite is true for the case where a majority are 'spin-down'. The system also exhibits a certain symmetry, whereby its energy is the same for when $s_{all} = -1$ and $s_{all} = 1$. Thus at equilibrium, the probability of –M is equivalent to +M.

2.2 Monte Carlo methods – the Metropolis algorithm

Much like Molecular Dynamics, Monte Carlo (MC) methods are a technique applied to problems requiring the simulation of many-body systems. In statistical mechanics, it can be applied to simulation of problems such as the Ising model. The basis of MC methods lies with the evaluation of integrals involving random sampling of an ensemble of points chosen from a known probability density function, within some phase space occupied by the system being simulated [5].

The Metropolis algorithm (or Metropolis MC) is thus a method for simulating the flipping of spin states within the system. Consider the system of spins, where one is chosen at random – the *i*-th spin, in the 'up' state. Let ΔE_i be the change in system energy caused by the chosen spin flipping from s_i to $-s_i$. Three outcomes are now possible:

- If there is a *decrease* in system energy where $\Delta E_i < 0$, the algorithm allows the change and $s_i \rightarrow -s_i$.
- If $\Delta E_i > 0$ and the energy *increases*, the change is allowed, subject to the probability $p_i = e^{-\frac{\Delta E_i}{k_B T}}$
- Else, the state change is rejected and s_i remains unchanged.

Running through this procedure once is an 'attempted flip', as the spin may or may not change. In the simulation, the Metropolis algorithm will be repeated *N* times, equal to the number of spin sites on the lattice; completing *N* attempted flips is then a single MC sweep.

As the simulation is allowed to run, the system will eventually reach a state where a particular microstate (the ensemble of points) will appear with estimated probability $p_{eq}(S)$. As the Metropolis MC generates a large number of microstates, equilibrium averages can be obtained by averaging over all microstates *S* [4].

For this system, the microstate contains all specified spin values, denoted by a capital *S* for the general microstate. At an arbitrary temperature T, the probability of finding the system in microstate *S* is understood to follow the equation

$$p_{eq}(S) = \frac{1}{Z(T)} e^{-\frac{E(s)}{k_B T}} \tag{6}$$

where *E(S)* is the microstate energy and k_B the Boltzmann constant. *Z(T)* is the partition function, summing over all possible microstates, expressed as

$$Z(T) = \sum_S e^{-\frac{E(s)}{k_B T}} \tag{7}$$

2.3 Treatment of errors

An important part of any study, and an indication of due scientific rigour, error analysis allows for formal justification of the obtained results and aids in future reproducibility of the research. For the purposes of this investigation, the standard deviation and standard error of the results will be considered, to 3 significant figures, via equations (8) and (9) respectively below [6]

$$\sigma_X = \left[\overline{X(t)^2} - \overline{X(t)}^2 \right]^{\frac{1}{2}} \tag{8}$$

$$\sigma_{\bar{X}} = \frac{1}{\sqrt{n-1}} \left[\overline{X(t)^2} - \overline{X(t)}^2 \right]^{\frac{1}{2}} \tag{9}$$

For a series of values $X_i(t)$, the average is given by $\overline{X(t)}$, measurements of some variable over a series of runs $i = 1 \ldots n$ in a time *t*,

$$\overline{X(t)} = \frac{1}{n} \sum_i X_i(t) \tag{10}$$

3. Investigative results

3.1 Convergence to equilibrium

From the base Ising Model code, the first set of modifications to the program introduced a function to calculate the magnetisation *M*. The system energy was also calculated, in the form of the dimensionless energy *E/J*. A code snippet is provided in Appendix (c). A key toggle was implemented with the 'm'-key, which would output the respective values to the console while the program window was open. A method was also implemented to write the magnetisation and dimensionless energy to an output file for each sweep.

The simulation was initialised with all spins aligned downwards, giving an initial value of $M = -1$ for the magnetisation. It was then run over 500 MC sweeps for a range of β-values (the inverse temperature) from 0.2 to 0.7 in steps of 0.05, on a 40x40 grid. A sufficiently large number of sweeps was chosen to allow the simulation to run for long enough to observe the system convergence to equilibrium.

For the same initial conditions at each β-value, 5 sets of data for both magnetisation and dimensionless energy were generated to determine the significance of random noise on the results. The data was then collated, and every 10th sweep plotted as a preliminary step, illustrated in figure 1. A full plot of all 500 sweeps may be found under Appendix (a). Comparing the

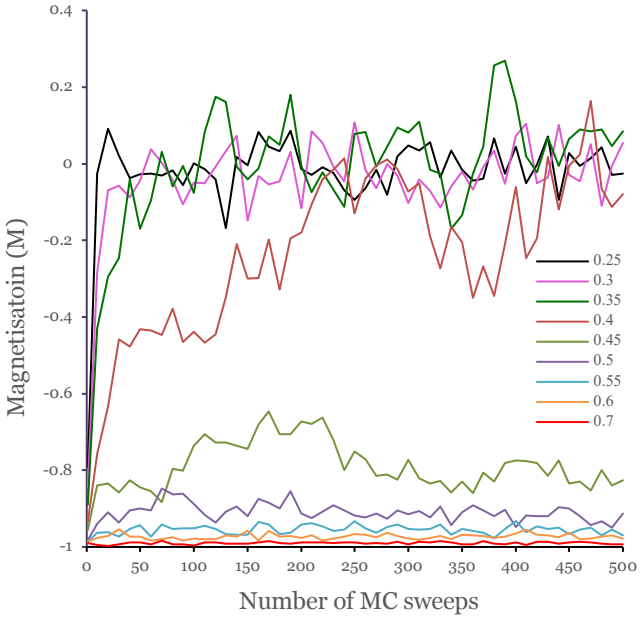


Figure 1: Visualisation of system magnetisation over a sample of β-values.

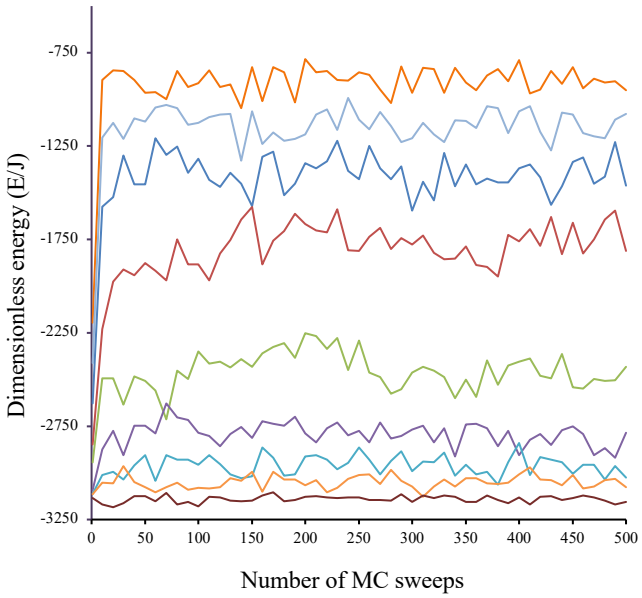


Figure 2: Overall dimensionless energy of the system for β = 0.2 to β = 0.7.

standard deviations of each plot in figure 1, the largest standard deviation was found to be ±0.18 at β = 0.4, with the smallest being ±0.007 from β = 0.6. The average over all plots was ±0.07. The standard error was the largest again for β = 0.4, at ±0.08, the average being ±0.03. Given the scale and amount of data points on figure 1, error bars were omitted as their scale would be negligible.

For β-values of 0.35 and below, figure 1 shows that the system rapidly converges to an equilibrium around M=0, consistent with disordered spin states, within less than 25 MC sweeps. An increase in the value of β was also correlated with an increase the number of time for the system to reach equilibrium. This might arise from the lower temperatures decreasing the spin-flip probability within the Metropolis algorithm. At a value of β = 0.4, the system was observed to require a greater number of sweeps needed to achieve equilibrium, first reaching M=0 around 250 MC sweeps and fluctuating for a further 100 sweeps before appearing to settle around 410 sweeps. At β = 0.45 and greater, the system was no longer observed to reach an equilibrium around M=0, tending to a value close to M=-1.

Hence it can be inferred that between the values of β = 0.4 and β = 0.45 the system undergoes a shift in its value of equilibrium. This is clearly depicted in figure 1, where the system begins to favour equilibrium in a magnetised state as β > 0.45. A more detailed visualisation of this trend is found in Appendix (a). This may also indicate that the system has undergone a phase transition as β increases from β = 0.4 to β = 0.5. The magnetisation at β = 0.5 still shows some tendency towards having some number of disordered spins, and appears to be the lower threshold of the transition. Referring equation 6, the probability of a spin flip increases with higher temperatures, consistent with a lower value of β. Lower temperatures have a greater chance for rejection of spin flips, thus resulting in magnetisation of the system.

Consideration of the energy of the system, illustrated in figure 2, further reinforces this notion. Less energetic systems have a lower tendency towards higher energy states, as shown by the smaller fluctuations at higher β-values. At lower β-values, the behaviour of the system energy follows a consistent trend, until it reaches the phase transition indicated in figure 1 between β = 0.4 to β = 0.5. This hypothesised phase transition is further supported by the large change in energy from β = 0.4 to β = 0.45.

As the overall system energy was considered, the largest standard deviation and standard error was in the order of ±94.9 and ±4.24 respectively, again from β = 0.4, with corresponding averages of ±65.1 and ±2.91. That β = 0.4 produced the largest errors was consistent with analysis of the magnetisation. As a matter of interest, a full plot of the dimensionless energy is provided in Appendix (b).

3.2 Equilibrium averages and comparison with mean-field theory; variation of system size

Use of the Metropolis MC also allows for determination of the system properties at equilibrium [4]. Once the system has reached an equilibrium, the simulation then creates *m* configurations to average over. The observables of the system are calculated – in this case, the energy and magnetisation – and from these an equilibrium average may be attained. For the Ising

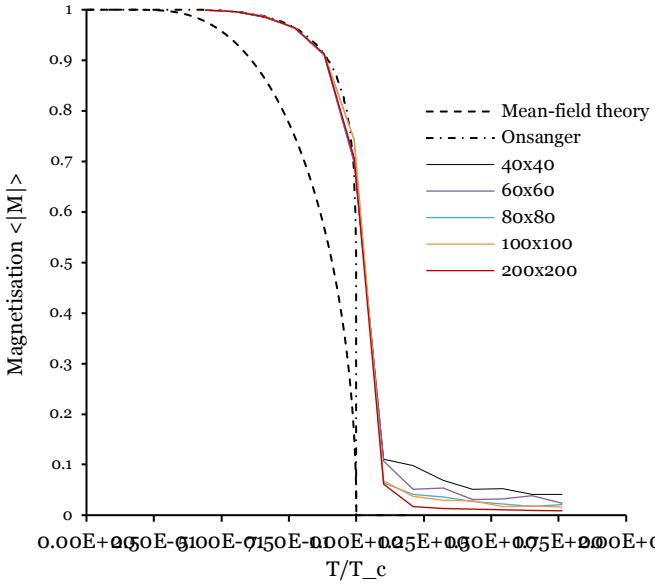


Figure 3: A comparison of the equilibrium averages for the absolute magnetisation against the predicted behaviour from the mean-field theory and Onsanger solution. Also pictured are results from different grid sizes.

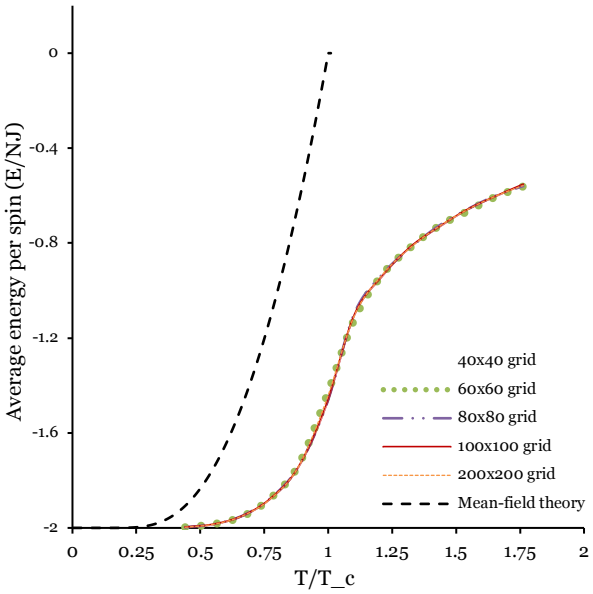


Figure 4: The equilibrium averages for the energy per spin, compared to the mean-field theory. Variation based on grid sizes was also investigated.

model, the phase-space volume involved is still within a suitable size to apply the use of time-averaging [4]. More complicated systems tend to have prohibitively large phase space volumes, making them difficult to fully investigate within available simulation time. In such cases, time-averaging is replaced by averaging over all ensembles in the system [5]. To facilitate this section of the investigation, the simulation was further modified with a method that now discarded the first n_o MC sweeps, effectively the amount of time the simulation should 'wait' before taking measurements, allowing it to reach a steady state. The method was then run for a number of measurements m, at intervals of n MC sweeps (equivalent to $n_0 + nm$ MC sweeps in total); the average values of the magnetisation, absolute magnetisation and energy per spin were calculated and written to an output file. These measurements were obtained for a dimensionless temperature T_o, between values of 1.0 and 4.0.

The number n_o was chosen based on results from section 3.1; approximately 250 MC sweeps were needed before the system reached an equilibrium at each value of β. Based on an informed estimate and some trial-and-error, 50 measurements at intervals of 20 MC sweeps was found give a balance between quantity of results and simulation time. As such, the simulation only required 30 seconds on average for grid sizes up to and including 100x100; 2 minutes were needed to record all measurements for a 200x200 grid

From figure 3, the absolute equilibrium averages for magnetisation of the system exhibit an approximately constant value of M=1 until around 0.8T/T_c, after which the plot instantaneously drops to a value close to M=0, at the boundary of 1T/T_c. This temperature is understood to be the critical temperature, characterised by the material beginning to approach its Curie temperature. Comparing this result to the mean-field approximation shows that the drop-off to M=0 occurs at a much lower temperature than the simulation results. Where the simulation displays a more gradual tend towards M=0, the mean-field approximation is discontinuous at the critical temperature. This discontinuity is also exhibited by the plot produced from the Onsanger solution. There is agreement between the simulation results and Onsanger solution during the initial drop-off; however, as the magnetisation approaches 0, the results begin to diverge, but with the results from grid sizes of 100x100 and 200x200 showing the closest fits. Referring to the theory [4], this can be explained by the fact that the Onsanger solution is only valid for very large lattices.

The comparative difference of the mean-field theory in this regard may be attributed to the assumption that it makes to neglect the correlations between spins, treating them as being within an identical setting, and using the concept of a 'mean field', $\langle h_i \rangle$. However, as discussed in section 2.1, h_i denotes the local field for the i-th spin in the Ising model. This strong assumption thus results in a model that assumes a system akin to a 'one-body model', that breaks down as it approaches the critical temperature.

Considering next the plots for equilibrium averages for the spin energy, the discrepancies of the mean-field are even more apparent, as shown in figure 6. The Ising model results for different grid sizes are extremely

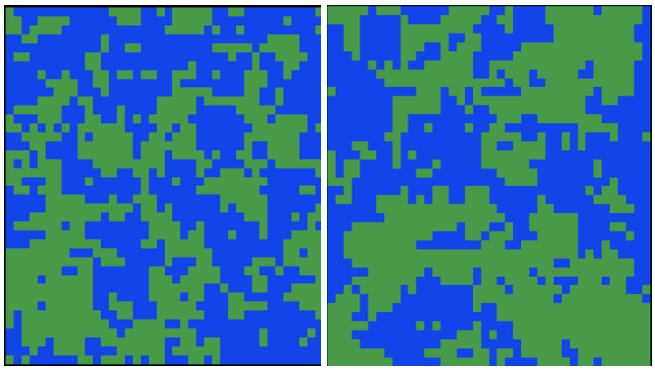


Figure 5: Samples of the Ising model system at equilibrium, showing spin clusters at $\beta = 3.5$ (left) and $\beta = 4$ (right). Both are 40x40 grids.

Figure 6: Two interesting examples of hysteresis encountered. The left image is taken at equilibrium for a 200x200 lattice, at $\beta = 5.6$. The image on the right was from a 40x40 grid, $\beta = 1.6$.

similar, with the energies all closely following the same pattern, and beginning to increase at around $0.5T/T_c$. The energies from the mean-field theory instead increase from around $0.25T/T_c$, and increase somewhat asymptotically with temperature towards 0 energy, appearing to not cross $1T/T_c$. Again, this stems from the crucial assumption made by the mean-field theory. In the case of the energy predicted by this theory, by ignoring the individual contribution from each individual local spin field, the theory is only able to model the overall alignment of the system. Whereas the Ising model instead has a turning point at the critical temperature, and takes into account the effect from clusters of similarly-aligned spins. An example of these clusters is found in figure 5, with larger clusters of such spins present at $\beta = 4$.

3.3 A brief look at hysteresis

As with elastic materials, magnetic systems can also exhibit hysteresis; in the Ising model, heating an initially cold system and subsequently cooling it back to its original temperature can result in the system no longer returning to its preliminary state.

Due to time constraints, the entirety of this feature was not able to be investigated, however, several results were observed, evidence that the simulation was capable of exhibiting hysteresis. These are pictured in figure 6.

4. Conclusion

Though simple theory, computational implementation of the Ising model found to provide robust simulations of s system of spins. The use of Metropolis Monte Carlo provided a suitable method for inducing spin flips in the system, as well as determination of the averages for system magnetism and energy per spin at equilibrium though time-averaging.

Observation of system trends to equilibrium for magnetisation and overall energy over a range of β-values were discussed in section 3.1, visualised in figures 1 and 2. A larger β-value was seen to correlate with an increased time for equilibrium to be reached, consistent with a lower system temperature. Indication of a phase transition within the system was also seen between $\beta = 0.4$ and $\beta = 0.5$. The largest standard errors and standard deviations were obtained from plots at $\beta = 0.4$, for both magnetisation and energy.

Comparison of the Ising model simulation results to other theories such as the mean-field approximation and exact Onsanger solution was discussed in section 3.2. The simulation was found to be in good agreement with behaviour predicted by the Onsanger solution, with the closest fit observed at larger grid sizes. However, the mean-field approximation predicted quite different patterns of behaviour from that of the Ising model, most prominently in the region approaching the critical temperature. This was understood to arise from several key assumptions in mean-field theory, namely the treatment of spins as individualistic, and taking a 'mean field' for the spin magnetisation.

References:

[1] Niss, M., 2009. History of the Lenz–Ising Model 1950–1965: from irrelevance to relevance. *Archive for history of exact sciences*, *63*(3), p.243.

[2] Brush, S.G., 1967. History of the Lenz-Ising model. *Rev. of mod. Phys.*, *39*(4), p.883.

[3] James, R., 2018. PH30031 Simulation Techniques, Lecture 7 The Monte Carlo Method (MC). University of Bath.

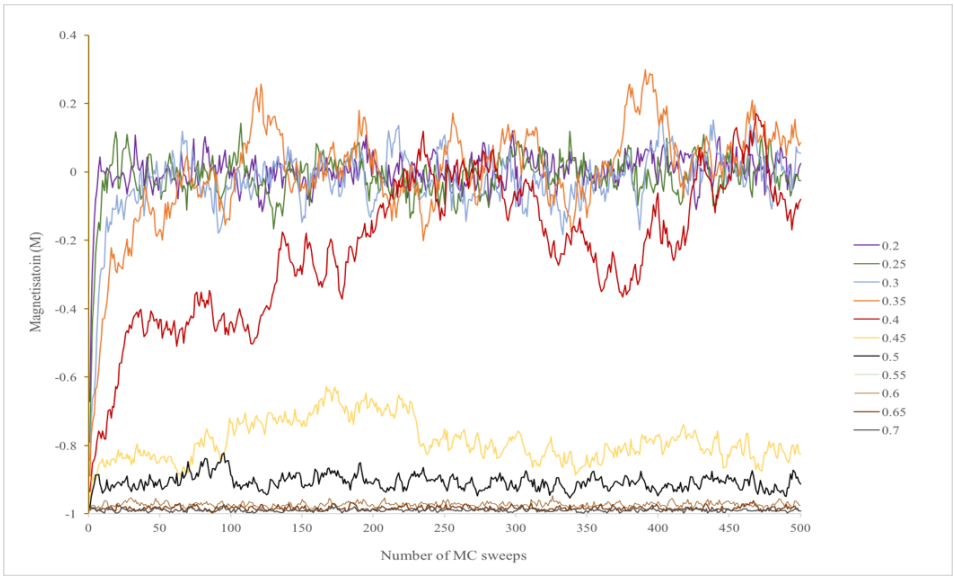
[4] Rimpilainen, V. J. T., 2018. PH30056 Computational Physics B, Ising Model Coursework Assignment. University of Bath.

[5] James, R., 2018. PH30031 Simulation Techniques, Lecture 6&7 Simulation of many-body systems. University of Bath.

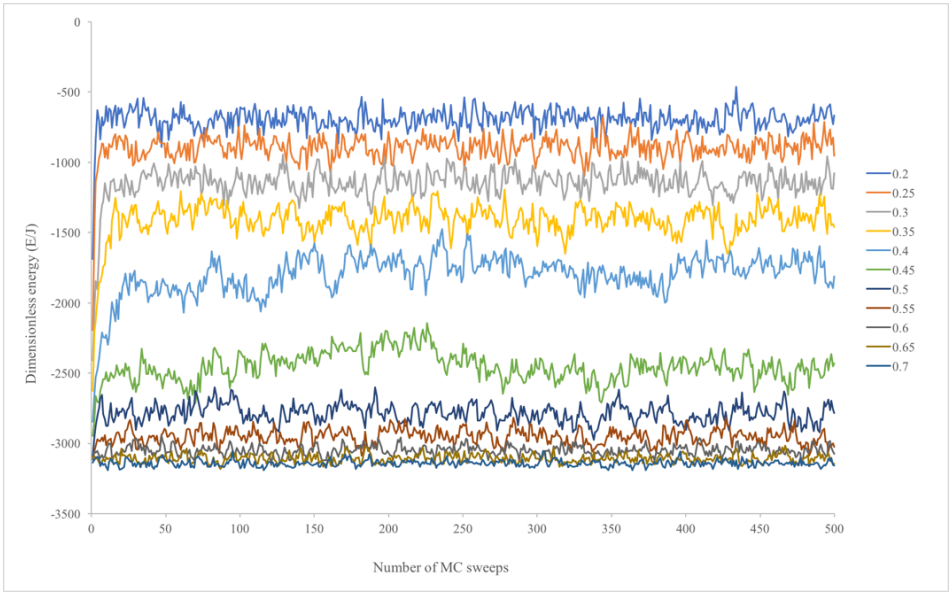
[6] Rimpilainen, V. J. T., 2018. PH30056 Computational Physics B, Lecture 4. University of Bath.

Appendix

a) Full plots of system magnetisation over a range of β-values from 0.2 to 0.7.



b) Full plots of system dimensionless energy over a range of β-values from 0.2 to 0.7.



c) Code snippet for calculation of magnetisation and overall system energy:

```
double IsingSystem::calculateMagnetisation() {
    double M = 0;
    double mag;
    //const double N = gridSize*gridSize;

    for (int x = 0; x < gridSize; x++) {
        for (int y = 0; y < gridSize; y++) {
            int posArray[2] = {x, y};
            M += readGrid(posArray);
        }
    }

    mag = M/(gridSize*gridSize);
    return mag;
}

double IsingSystem::calculateDimensionlessE() {
    double ans = 0;

    for (int x = 0; x < gridSize; x++) {
        for (int y = 0; y < gridSize; y++) {
            int pos[2] = { x, y};
            double innerSum = 0;

            for  (int a = 0; a < 4; a++) {
                int neighbourPos[2];
                setPosNeighbour(neighbourPos, pos, a);
                innerSum += readGrid(neighbourPos);
            }

            innerSum *= -readGrid(pos);
            ans += innerSum;
        }
    }

   return ans *= 0.5;
}
```