

Computational Many Body Physics: Part 2

The Ising Model

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Abstract

This project studies the two-dimensional Ising model using Monte Carlo simulations. The system is initialized with random spin configurations and evolved using both the single-spin Metropolis algorithm and a cluster-flip algorithm based on the Wolff method. We visualize the evolution of spin configurations, study convergence towards equilibrium, and compare the efficiency of the two updating schemes. Autocorrelation effects are quantified using a binning analysis of the magnetisation, allowing estimation of statistical errors and autocorrelation times. We investigate the dependence of magnetisation on temperature for different lattice sizes and observe a clear signature of the ferromagnetic-paramagnetic phase transition. The autocorrelation time is studied as a function of temperature, revealing critical slowing down in the Metropolis algorithm and a significant reduction of autocorrelation times for the Wolff algorithm. Finally, the specific heat is computed from energy fluctuations and exhibits a pronounced peak near the critical temperature, consistent with the expected phase transition of the two-dimensional Ising model.

1 Introduction

The Ising model is a paradigmatic model in statistical physics used to study phase transitions and critical phenomena. It consists of discrete spins $s_i = \pm 1$ placed on a lattice, interacting with their nearest neighbours. Despite its simplicity, the two-dimensional Ising model exhibits a non-trivial phase transition between an ordered ferromagnetic phase and a disordered paramagnetic phase.

In this project, Monte Carlo methods are employed to study the equilibrium and dynamical properties of the two-dimensional Ising model. The single spin-flip Metropolis algorithm and the Wolff cluster algorithm are implemented and compared. Quantities such as magnetisation, autocorrelation time, and specific heat are measured to characterise the phase transition and algorithmic efficiency.

2 Ising Model and Monte Carlo Algorithms

The Hamiltonian of the two-dimensional Ising model is given by

$$H = - \sum_{\langle i,j \rangle} s_i s_j, \tag{1}$$

where $s_i = \pm 1$ and the sum runs over nearest-neighbour pairs. Periodic boundary conditions are used throughout this work.

2.1 Single Spin-Flip (Metropolis) Algorithm

In the Metropolis algorithm, a single spin is selected and flipped with probability

$$P = \min\left(1, e^{-\beta\Delta E}\right), \quad (2)$$

where ΔE is the energy change associated with the proposed flip and $\beta = 1/T$ is the inverse temperature. A Monte Carlo sweep corresponds to attempting updates at all lattice sites.

2.2 Wolff Cluster Algorithm

The Wolff algorithm constructs clusters of aligned spins that are flipped collectively. Starting from a randomly chosen seed spin, neighbouring spins with the same orientation are added to the cluster with probability

$$p = 1 - e^{-2\beta}. \quad (3)$$

Flipping entire clusters significantly reduces critical slowing down near the phase transition.

3 System Evolution and Convergence

Starting from a random initial configuration, the system evolves towards equilibrium under repeated Monte Carlo updates. At low temperatures, large ferromagnetic domains form, while at high temperatures the system remains disordered.

Figure 1 compares the convergence of the absolute magnetisation for the Metropolis and Wolff algorithms at low temperature. The Wolff algorithm reaches equilibrium much faster than the Metropolis algorithm due to its non-local updates.

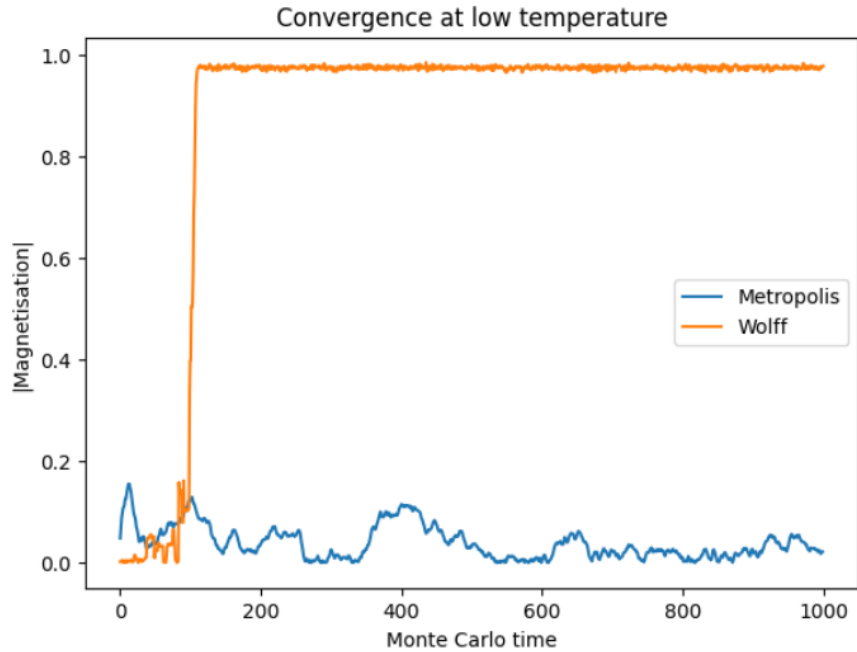


Figure 1: Convergence of the absolute magnetisation at low temperature for the Metropolis and Wolff algorithms.

4 Binning Analysis and Autocorrelation

Monte Carlo measurements are correlated, leading to an underestimation of statistical errors if correlations are ignored. To account for this, a binning analysis was performed by successively averaging neighbouring data points and evaluating the standard error of the magnetisation.

As the bin size increases, the estimated error initially grows and eventually saturates, indicating that correlations have been properly taken into account. Over-binning results in noisy estimates due to insufficient statistics.

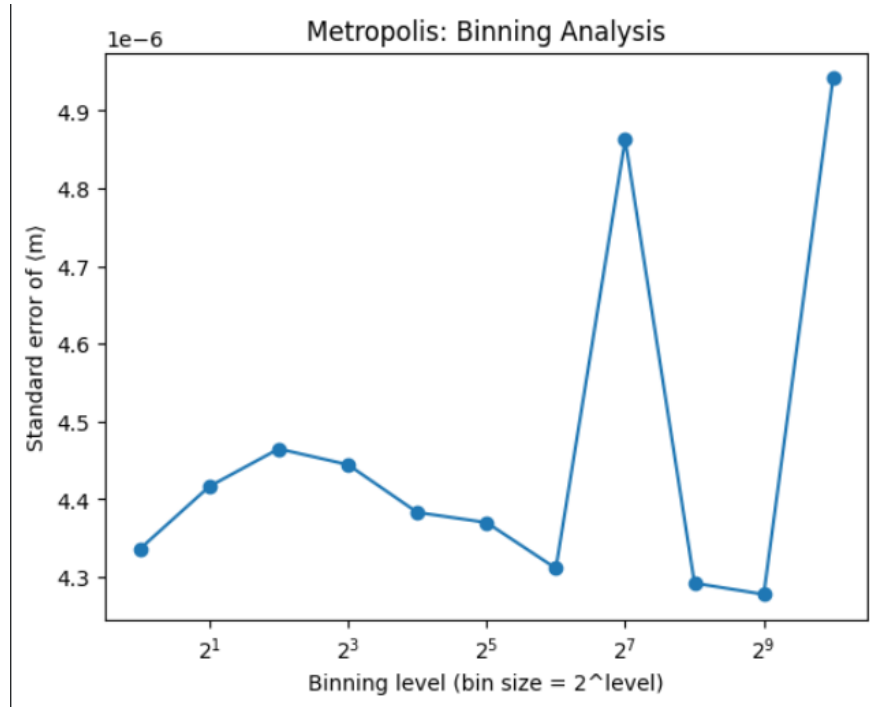


Figure 2: Binning analysis for the Metropolis algorithm.

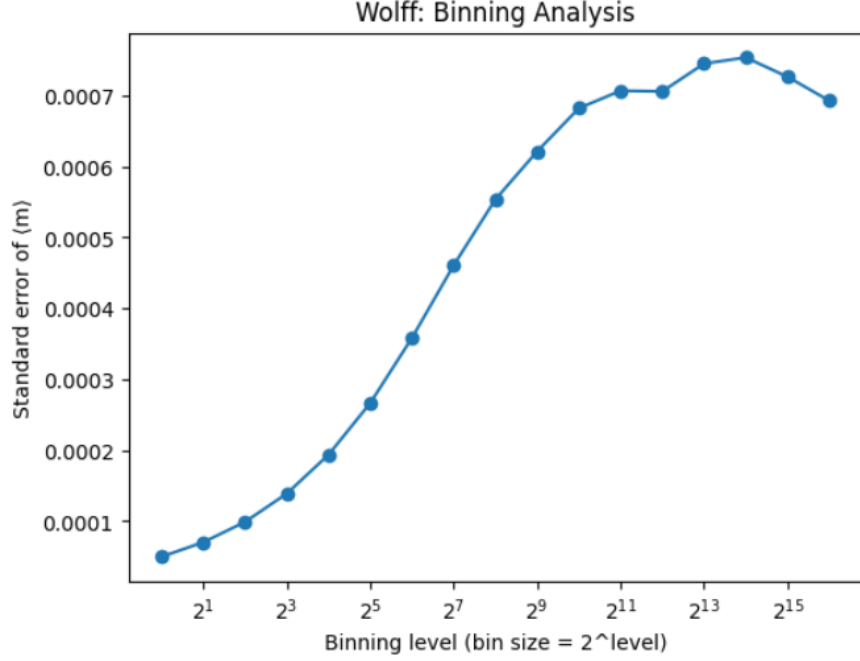


Figure 3: Binning analysis for the Wolff algorithm.

5 Magnetisation as a Function of Temperature

The equilibrium magnetisation was measured as a function of temperature for lattice sizes $L = 8, 10$, and 12 . To avoid cancellation due to symmetry between positive and negative magnetisation states, the absolute magnetisation $\langle |M| \rangle$ was used.

Figure 4 shows a sharp decrease in magnetisation near $T \approx 2.3$, indicating a phase transition from an ordered to a disordered phase. The transition becomes sharper with increasing lattice size, consistent with finite-size scaling.

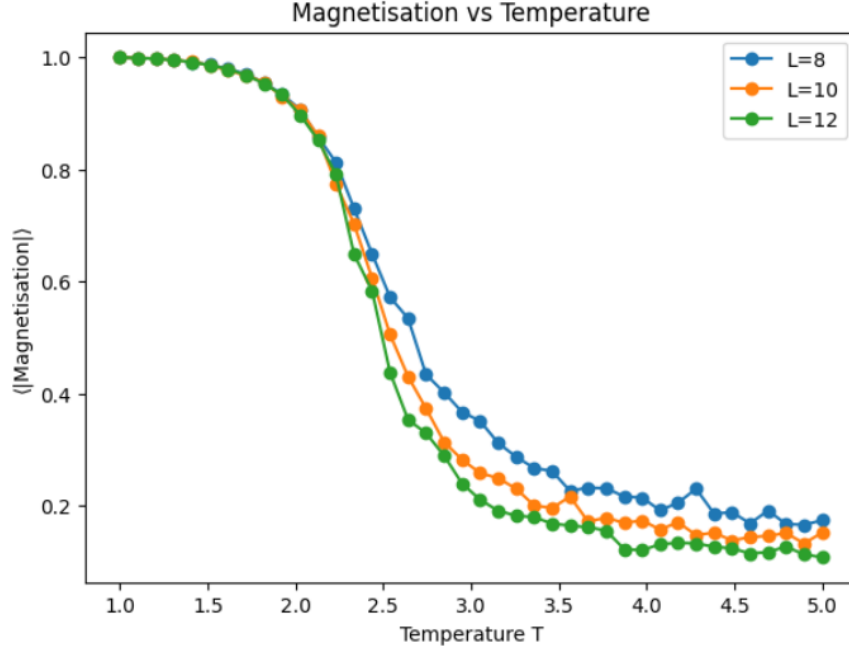


Figure 4: Magnetisation as a function of temperature for different lattice sizes.

6 Autocorrelation Time as a Function of Temperature

The autocorrelation time of the magnetisation was computed as a function of temperature for both the Metropolis and Wolff algorithms. The autocorrelation time measures how quickly statistically independent configurations are generated.

Figure 5 shows a pronounced peak in autocorrelation time near the critical temperature for the Metropolis algorithm, indicating strong critical slowing down. In contrast, the Wolff algorithm exhibits significantly reduced autocorrelation times across all temperatures, demonstrating its effectiveness in overcoming critical slowing down.

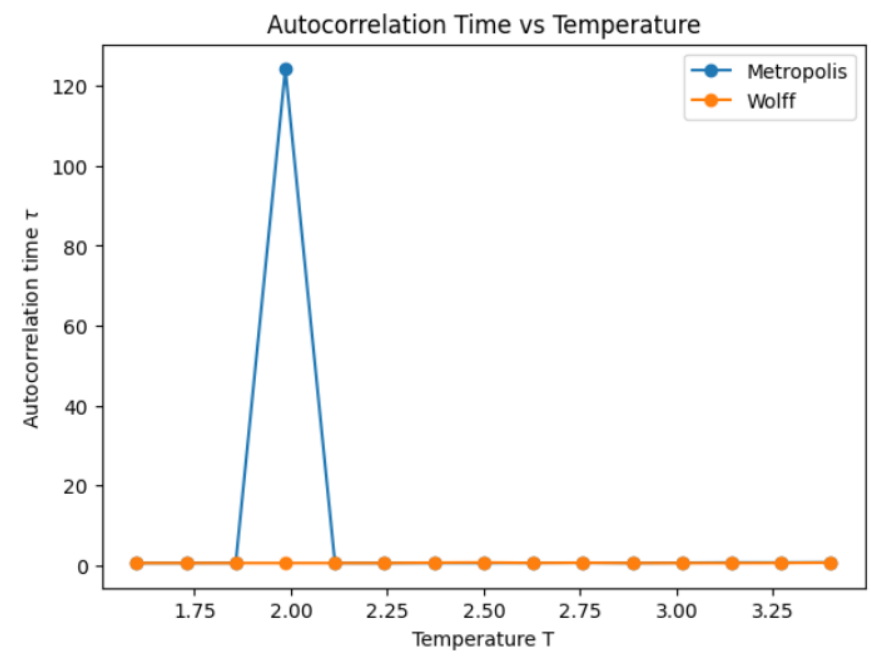


Figure 5: Autocorrelation time as a function of temperature for Metropolis and Wolff algorithms.

7 Specific Heat

The specific heat was computed using

$$C_V = \frac{\langle E^2 \rangle - \langle E \rangle^2}{NT^2}, \quad (4)$$

where N is the total number of spins. A peak in the specific heat is observed near the critical temperature. The peak sharpens with increasing lattice size, providing further evidence for the phase transition.

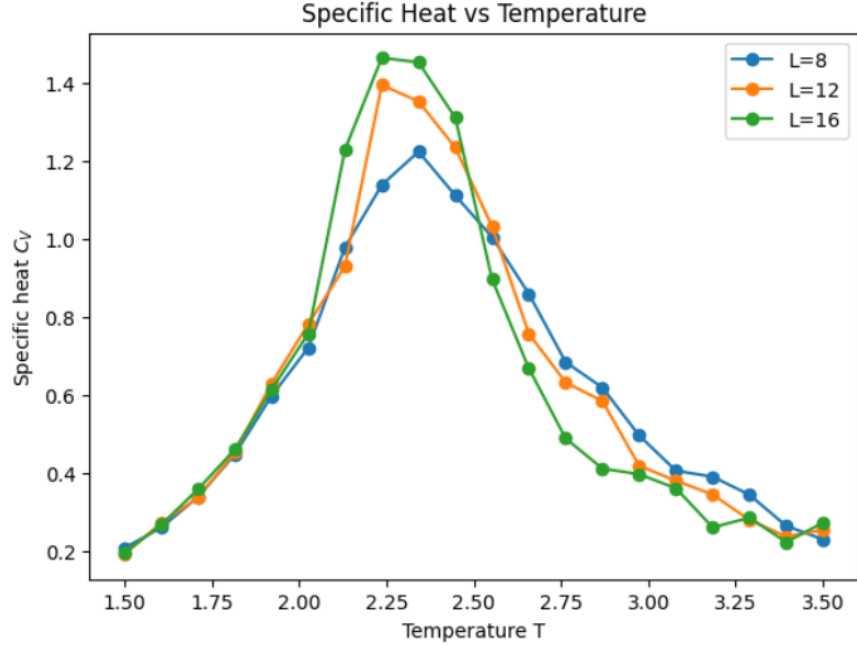


Figure 6: Specific heat as a function of temperature for different lattice sizes.

8 Conclusion

In this work, Monte Carlo simulations were used to study the two-dimensional Ising model. The Wolff cluster algorithm was shown to outperform the single spin-flip Metropolis algorithm, particularly near the critical temperature, by significantly reducing autocorrelation times. Measurements of magnetisation, autocorrelation time, and specific heat consistently indicate a phase transition near $T \approx 2.3$, in agreement with theoretical expectations.

References

- [1] E. Luijten, “Introduction to Cluster Monte Carlo Algorithms,” *Lecture Notes in Physics*, **703**, 13–38 (2006).
- [2] S. Trebst, “Computational Many-Body Physics: Monte Carlo Methods,” Lecture notes, University of Cologne (2025). Available at: <https://www.thp.uni-koeln.de/trebst/Lectures/2025-CompManyBody.shtml>