

# Phase Transitions and the Ising Model

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## Introduction

The purpose of this paper is to report on the results of multiple simulations pertaining to phase transitions in two-dimensional spin lattices. All lattices studied were square and contained only spin  $\frac{1}{2}$  particles. The simulations investigated...

The simulations were coded in FORTRAN90.

We will first discuss the physics of the Ising model. Then, we will discuss the multiple algorithms used to study the Ising model. Finally, we will investigate specific results of the simulations.

## The Ising Model

The purpose of the Ising model is to describe the dynamics of phase transitions in ferromagnetic materials. The one-dimensional Ising model, which has no phase transitions, was solved by Ernst Ising in 1925. The two-dimensional square lattice Ising model was analytically studied by Lars Onsager in 1944.

In the Ising model, the Hamiltonian of a spin  $\frac{1}{2}$  ferromagnet of a general shape is

$$H = -J \sum_{ij} S_i S_j$$

where  $J > 0$  is a ferromagnetic exchange constant,  $S_i = \pm 1$  is a spin variable, and the summation is over the nearest-neighbor sites on the lattice.

The quantity that characteristically describes any magnet is the magnetization  $m$ , which is defined as

$$m = \frac{\sum_i S_i}{N}$$

where  $N$  is the total number of spin particles in the ferromagnet.

The properties of all magnetic materials change as a function of the temperature of the material. A quantity of interest is the Curie temperature

$T_c$ , which is defined as the temperature at which a magnetic material loses its permanent magnetism. In other words, at  $T_c$  an “order-to-disorder” phase transition occurs in the orientations of the spins of the ferromagnet. At temperatures higher than  $T_c$ , the magnet is very susceptible to induced magnetization.

## Monte Carlo Methods

The analytical description of the Ising model is impractical to use because transitions near  $T_c$  exhibit complex phenomena. In light of this, the Ising model has been extensively studied by use of Monte Carlo methods.

Monte Carlo methods were first studied during the Manhattan project in the 1940s and serve to deepen our theoretical understanding of physical phenomena.

### Metropolis Algorithm

The Metropolis Algorithm was first published in 1953 and is considered to be the most widely used Monte Carlo algorithm. Simply put, it is a method for obtaining a sequence of random values from a probability distribution. This sequence can be used in numerous applications such as approximation of multi-dimensional distributions, numerical integration, and graph theory.

The outline of the mainloop of Metropolis algorithm, as applied to the Ising model, is as follows:

- (i) Randomly choose a location in the lattice randomly.
- (ii) Calculate the energy difference  $\delta E$  between the spin up and spin down orientations.
- (iii) Calculate the expression  $e^{\beta\delta E}$
- (iv) Let  $x$  be a random number on the interval  $[0, 1]$ . If  $e^{\beta\delta E} > x$ , then flip the randomly selected spin.
- (v) Calculate the magnetization by averaging over the orientation of all spins.

(vi) If satisfied with the value for the magnetization, exit the loop. If not satisfied, return to (i).

The above loop iterates over arbitrary time steps. After some time, the value for the magnetization should converge to a “small” range of values. The size of this “smallness” is determined by the needs of the experimenter.

### Cluster Algorithms

In the above Metropolis algorithm, one randomly selected spin is updated (flipped or not flipped) for each sweep across the entire spin lattice, which is computationally expensive. Also, at temperatures near the critical temperature, there is a large increase in fluctuations in total magnetization and total energy, which requires more measurements to reduce the statistical noise.

In the late 1980s, research began on new algorithms that would reduce the two issues stated in the previous paragraph. This would be achieved by updating clusters of spins for each sweep across the lattice. In these methods, the difficulty is in creating a method that efficiently and effectively identifies the appropriate clusters to be updated. In the case of the Ising model, the clusters are continuous groups of particles with the same spin orientation.

### Wolff Algorithm

In the Wolff algorithm, a single cluster is updated for each sweep of the lattice.

The outline of the algorithm as it is applied to the Ising model is as follows:

- (i) Randomly choose a location in the lattice randomly.
- (ii) There are eight nearest-neighbor locations to the randomly selected location. Choose a nearest-neighbor location of the same orientation as the spin in the first selected location. The choice does not have to be random.
- (iii) Let  $x$  be a random number on the interval  $[0, 1]$ . If  $1 - e^{\frac{2J}{u\beta T}} > x$ , then add the nearest-neighbor spin to the cluster.
- (iv) After growing the cluster to completion, flip the cluster.

(v) Continue

### Swendsen-Wang Algorithm

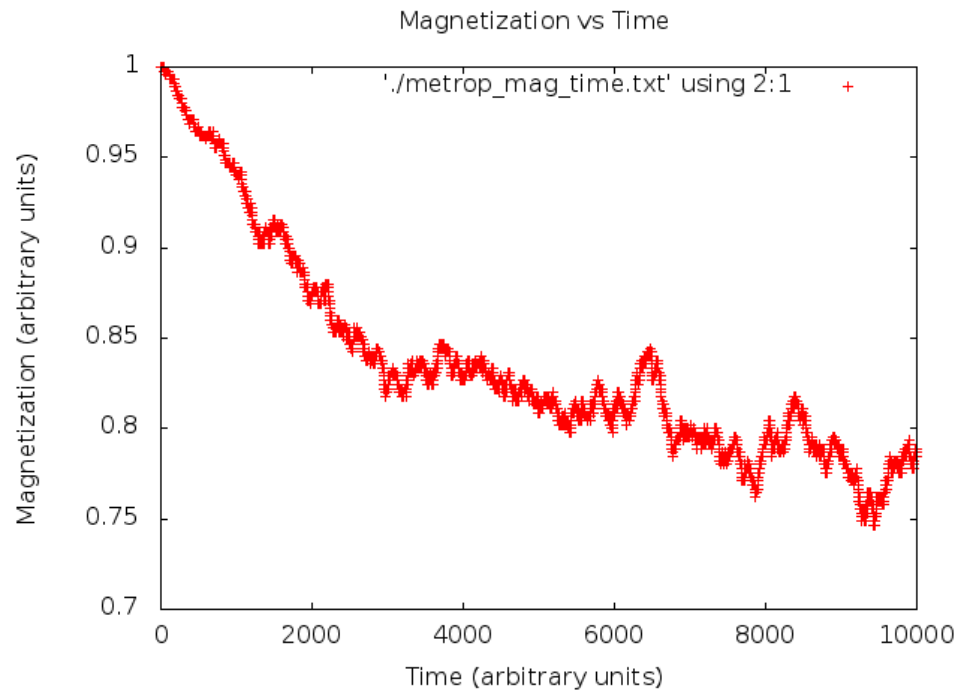
Unlike the Wolff algorithm, the Swendsen-Wang algorithm updates multiple clusters for each sweep of the lattice.

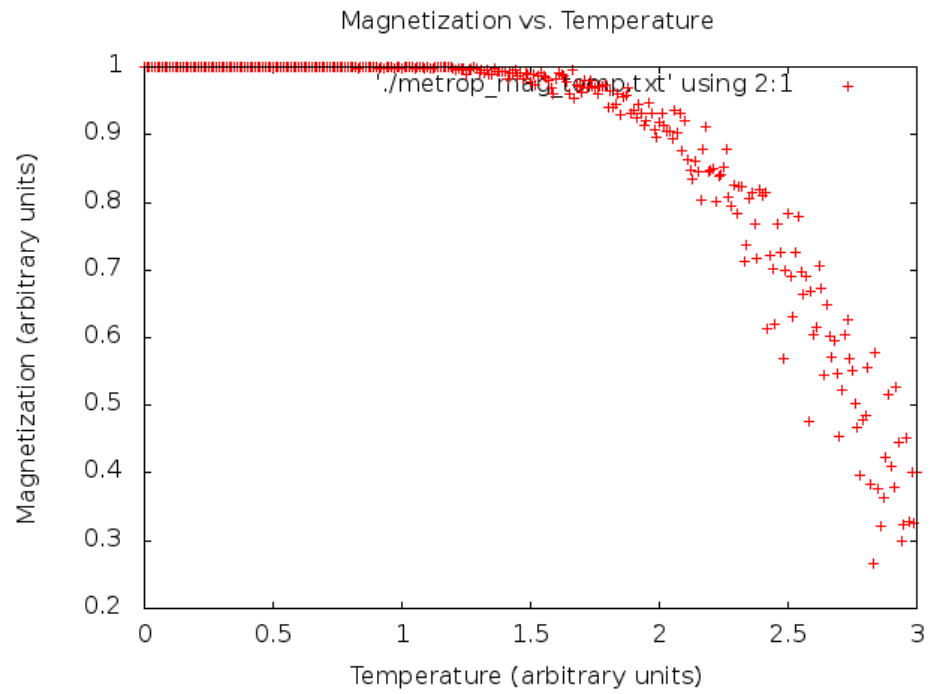
## Simulations and Results

We ran simulations of the ising model for all three algorithms: Metropolis, Wolff, and Swendsen-Wang. The purpose of these simulations is to investigate the Magnetization as a function of both time and temperature for different computational algorithms.

### Metropolis Algorithm

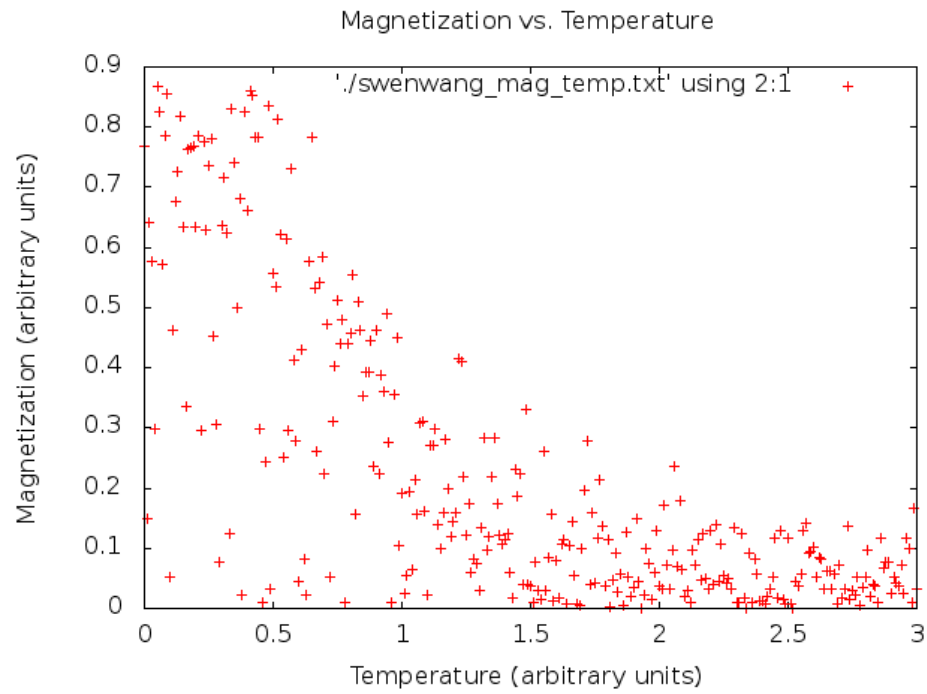
The following two plots are magnetization versus time and temperature respectively. For the temperature plot, a temperature of 2.5 was chosen. Note that the critical temperature is 2.3.





### Cluster Algorithms

The following plot is for the Swendsen-Wang Algorithm.



### Wolff Algorithm

The following plot is for the Wolff Algorithm.

