Computational Efficiency of the Metropolis and Wang-Landau Algorithms

Hanning Wong and Timothy Sullivan
Department of Physics, Kenyon College, Gambier OH

Abstract

Realistic atomic and molecular-scale simulations are computationally expensive, limiting the scope of applicable models. The focus of this research was to explore different computational methods in order to discover the methods that minimized the number of energy calculations required to characterize the thermodynamic properties of a ferromagnetic model. By using simplified models of a ferromagnetic system, we could compare the results of our research against established values. The Metropolis and Wang-Landau importance sampling algorithms were applied to the Ising and Heisenberg lattice models in order to provide comparative statistics. Four programs were generated comparing the Metropolis and Wang-Landau algorithm in two and three dimensions. The Metropolis algorithm required less energy computations than the Wang-Landau algorithm when both methods were used to compute energy as a function of inverse temperature to an accuracy of 5 percent. These results will be utilized to increase the computational efficiency of more realistic models.

Background

The Ising model is a mathematical model of ferromagnetism in statistical mechanics. This model can be used to model phase transitions of a ferromagnetic material as a function of changing temperature. The Ising model is comprised of a square lattice with N lattice sites, where each site contains a spin-1/2 particle that can have a spin magnetic moment of either +1 or -1 in scaled units. In order to reduce edge effects during simulations, periodic boundary conditions are employed. Any particular configuration of spins has a probability of occurring based on the Boltzmann distribution, where

$$P(\sigma) = \frac{e^{-\beta H(\sigma)}}{\sum_{\sigma} e^{-\beta H(\sigma)}}$$

The energy of the lattice for any configuration of spins is given by the Hamiltonian, where

$$H = -J \sum_{<i,j>} \sigma_i \sigma_j$$

The Hamiltonian sums over pairs of spins in a nearest neighbor system across the entire lattice, where J is the interaction strength between spins, commonly assumed to be 1 in scaled units. There are 2^N possible configurations in the Ising model, making it difficult to numerically evaluate thermodynamic averages for large lattices. Instead, methods such as the Metropolis Algorithm and the Wang-Landau algorithm allow thermodynamic statistics to be extracted from the model without needing to compute every possible configuration.

Metropolis Algorithm

The Metropolis Algorithm is a Monte Carlo Method that evaluates lattice configurations of the Ising Model based on their probability of occurring. The algorithm utilizes a quasi-random walk through phase space in order to simulate the random thermal fluctuation of the system from state to state over the course of an experiment [2]. All possible states are not evaluated during this method. Instead, an appropriate random set of states are generated according to the Boltzmann probability distribution through a chain of Markov processes. This Markov chain must satisfy the conditions of ergodicity and detailed balance in order to match the expected Boltzmann probability distribution of states. Ergodicity requires that every possible lattice configuration is accessible from any starting configuration and detailed balance requires that upon reaching equilibrium, the probability ratio of transitioning to and from any given configuration *u* is given by

$$\frac{P(\mu \to \upsilon)}{P(\upsilon \to \mu)} = e^{-\beta(E_\upsilon - E_\mu)}$$

Built around the principle of single-spin flip dynamics, each successive configuration is generated from a previous state using a transition probability that is dependent on the energy difference between the initial and final states. The algorithm randomly selects a lattice point and flips its spin state to the opposite value, and accepts the change based upon the most efficient acceptance ratio *A*, where

$$A(\mu \to \upsilon) = e^{-\beta(E_\upsilon - E_\mu)} \quad \text{for } E_\upsilon - E_\mu > 0$$
$$A(\mu \to \upsilon) = 1 \quad \text{for } E_\upsilon - E_\mu \leq 0$$

The algorithm repeats this process multiple times, creating a Markov chain that eventually reaches equilibrium, oscillating around a single energy value of the system that is equally likely to accept or reject a proposed spin configuration.

Wang-Landau Algorithm

The Wang-Landau Algorithm as applied to the Ising Model is another Monte Carlo Method that can be used to determine the thermodynamic properties of the system. The algorithm was designed to calculate the density of states, g(E), the number of all possible configurations for an energy level E of the system [3]. Unlike the Metropolis Algorithm, the Wang-Landau Algorithm does not evaluate the probability of a particular configuration at varying temperatures. Instead, the Wang-Landau Algorithm chooses its acceptance probabilities based on the reciprocal of the density of states at a given energy. The Wang-Landau Algorithm it must also satisfy the conditions of detailed balance and ergodicity during its random walk across configuration space in order to generate an accurate density of states function. During the simulation, single-spin flip dynamics occur as the system moves between configurations by proposing a single spin flip at a random lattice location. The transition probabilities between system energies before and after a spin value is changed is given by

$$p(E_1 \to E_2) = \frac{g(E_1)}{g(E_2)} \quad \text{for } g(E_1) \leq g(E_2)$$
$$p(E_1 \to E_2) = 1 \quad \text{for } g(E_1) \geq g(E_2)$$

The condition of ergodicity is clearly satisfied, since every configuration of spins is possible to reach by iterating through enough spin flips. In order to satisfy the condition of detailed balance, the ratio of transition probabilities to and from a single energy state upon reaching equilibrium must be

$$\frac{p(E_1 \to E_2)}{p(E_2 \to E_1)} = \frac{g(E_1)}{g(E_2)}$$

In the case of the Wang-Landau Algorithm, equilibrium is reached when an energy histogram tracking the system energy values visited is flat, meaning that all possible energy levels have been visited an equal number of times. This allows the algorithm to increase its accuracy of g(E) with subsequent iterations of smaller modifying factors to g(E). When the density of states has been calculated, statistics for all energy levels have been obtained, and various thermodynamic quantities can be calculated for any temperature.

Metropolis Data

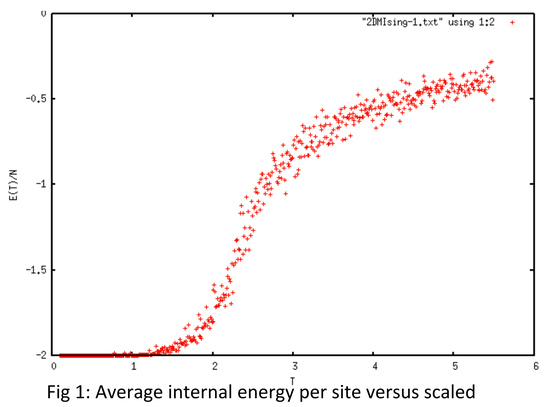

Fig 1: Average internal energy per site versus scaled temperature for 2D Ising model as calculated by the Metropolis Algorithm for lattice size L = 16

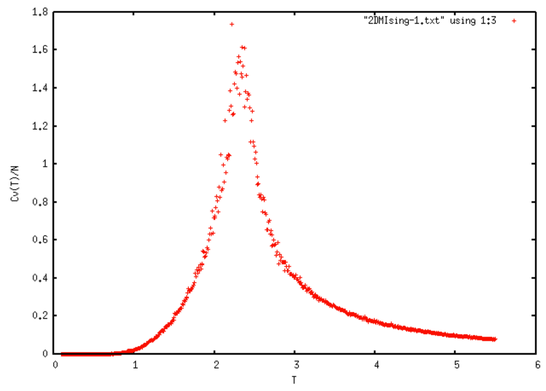

Fig 2: Average specific heat per site versus scaled temperature for 2D Ising model as calculated by the Metropolis Algorithm for lattice size L = 16

Metropolis Data

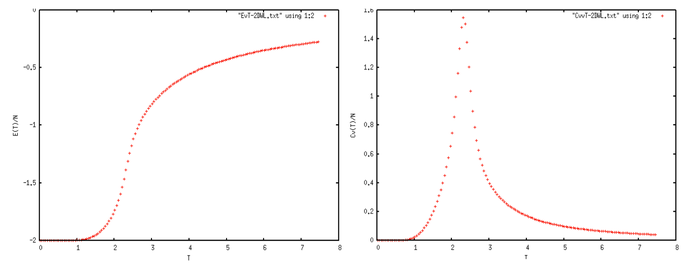

Fig 3: Average internal energy per site versus scaled temperature for 2D Ising model as calculated by the Wang-Landau Algorithm for lattice size L = 16.
Fig 4: Average specific heat per site versus scaled temperature for 2D Ising model as calculated by the Wang-Landau Algorithm for lattice size L = 16.

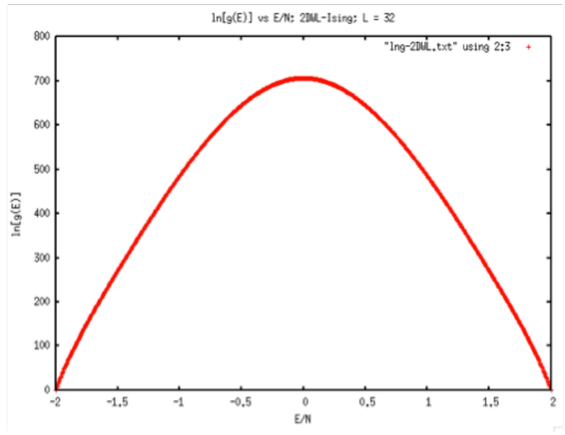

Fig 5: Logarithm of density of states, ln[g(E)] versus energy per site for the 2D Ising model as calculated by the Wang-Landau Algorithm for lattice size L = 16

Results

Four programs were generated comparing the Metropolis and Wang-Landau algorithm in two and three dimensions. These algorithms were both able to produce statistics on thermodynamic quantities including internal energy per site and specific heat per site. The number of energy computations required to characterize these quantities over a temperature range of 0.2Tc to 5.0Tc were compared between algorithms. For a L = 16 lattice, the Wang-Landau algorithm required on average 650 million energy calculations of the system in order to produce characteristic data within an accuracy of 5 percent, nearly 30 times more than the Metropolis Algorithm. From this, we conclude that the Metropolis algorithm is a more efficient method of characterizing ferromagnetic systems.

References and Acknowledgments

[1] Binder, K., and Dieter W. Heermann. *Monte Carlo Simulation in Statistical Physics: An Introduction*. Berlin: Springer-Verlag, 1988.
[2] Landau, David P., and K. Binder. *A Guide to Monte Carlo Simulations in Statistical Physics*. Cambridge: Cambridge UP, 2000.
[3] Newman, M. E. J., and G. T. Barkema. *Monte Carlo Methods in Statistical Physics*. Oxford: Clarendon, 1999.
[4] Landau, D.P, Shan-Ho Tsai, M. Exler, Am. J. Phys. **72** (10) October 2004

Many thanks to Professor Sullivan and the Kenyon Physics Department for making this project possible.