Monte Carlo Simulations: 2D Ising Model

Allen Poon **Dr. Ken D. Jordan**

First Experiences in Research, Dietrich School of Arts & Sciences, University of Pittsburgh

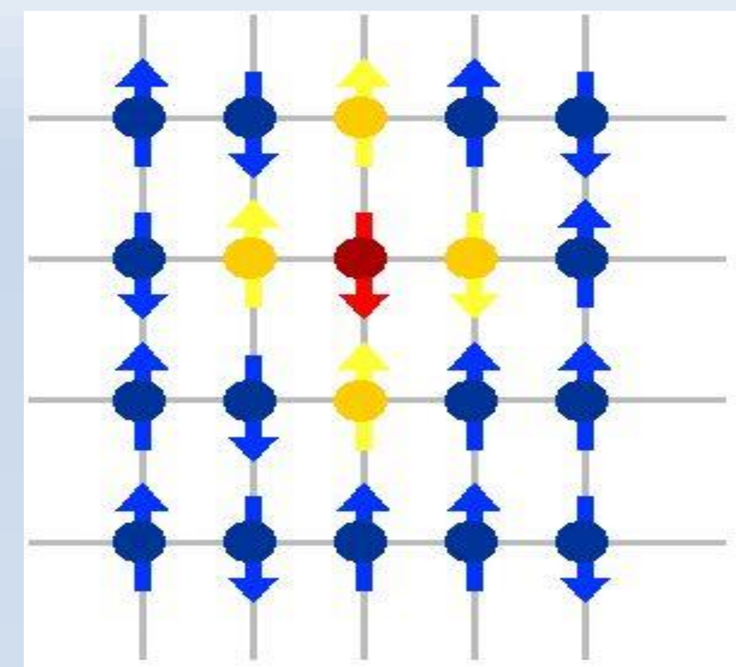
Introduction

- The Monte Carlo methods is a probabilistic algorithm involving importance sampling. Each step attempts to make a change based on the new energy versus the old
  - If $\Delta E \leq 0$, make the change
  - If $\Delta E > 0$, the change has a probability $e^{-\Delta E/k_b T}$ of being accepted
- 2D Ising Model implementation using the Metropolis-Hastings algorithm
  - Used for phase transitions such as ferromagnetism in this case
- The Ising model features magnetic moments of spins that can either be up (+1) or down (-1) arranged in a lattice where each interacts with its 4 nearest neighbors
  - The boundary condition holds so that the neighbor of the last spin on the right side is the first spin on the left side
  - $\Delta E = 2J * spin[i][j] * (spin_{left} +$

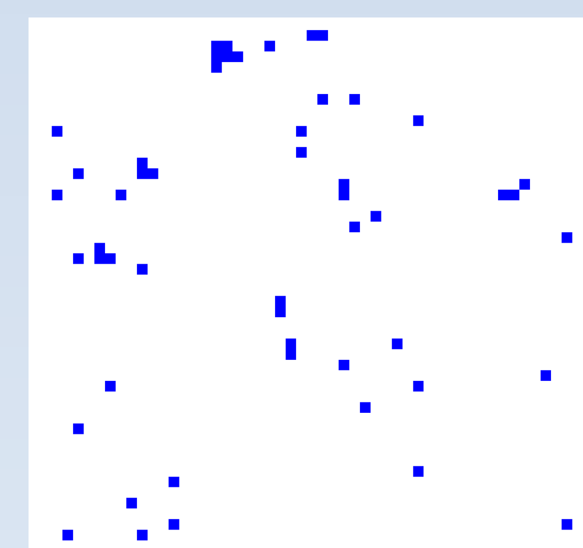
Methods

- Explore 2D Ising Model problem using a 50x50 lattice
  - Initialize lattice with random spins
  - For every temp, calculate the total energy and magnetization of the system
  - Equilibrate by running the simulation enough times
  - Continue simulation by accumulating data for energy and magnetization

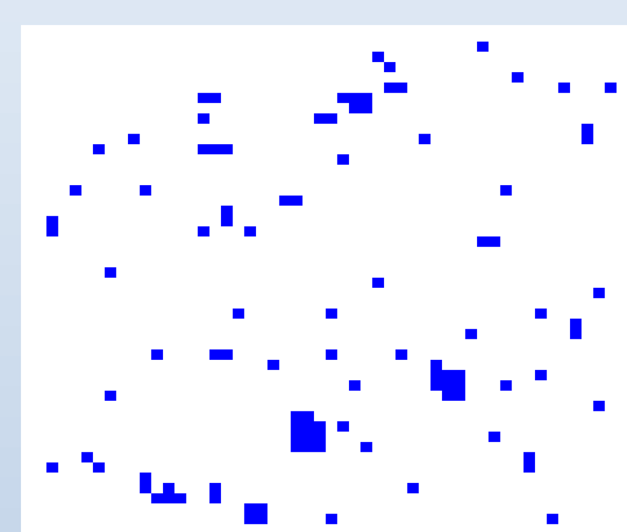
Results



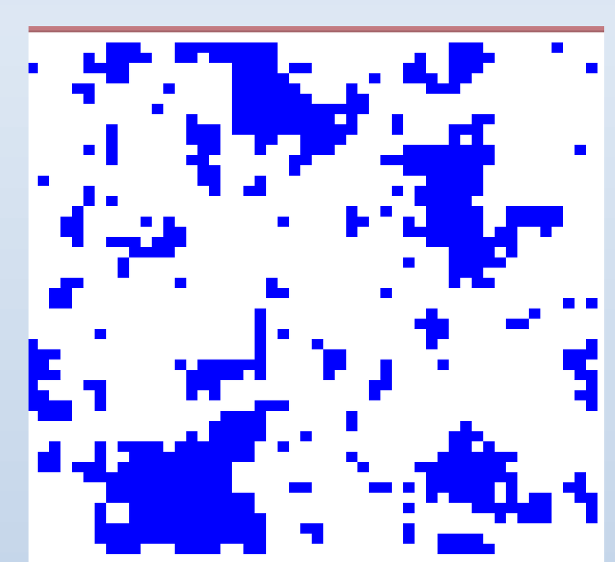
Random Config. Start



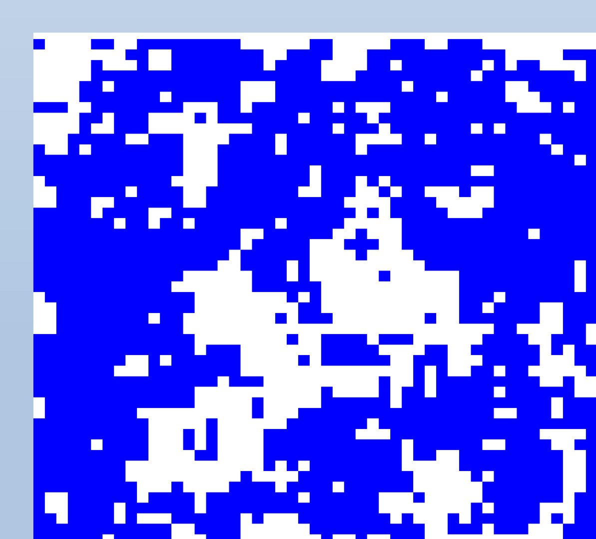
Temp = 1.82 J



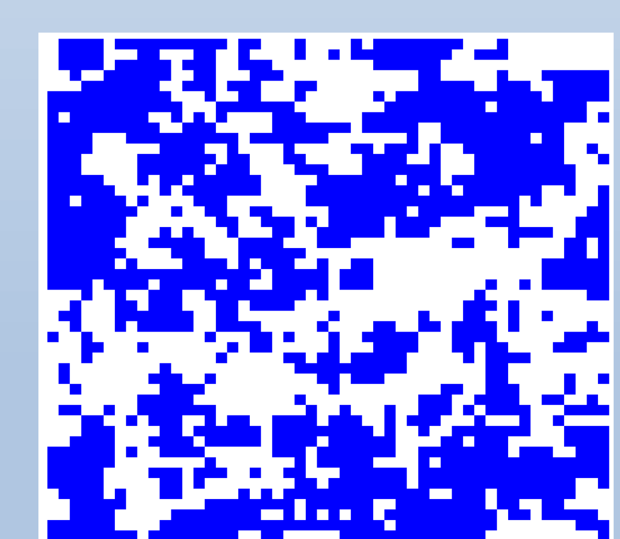
Temp = 2.04 J



Temp = 2.27 J



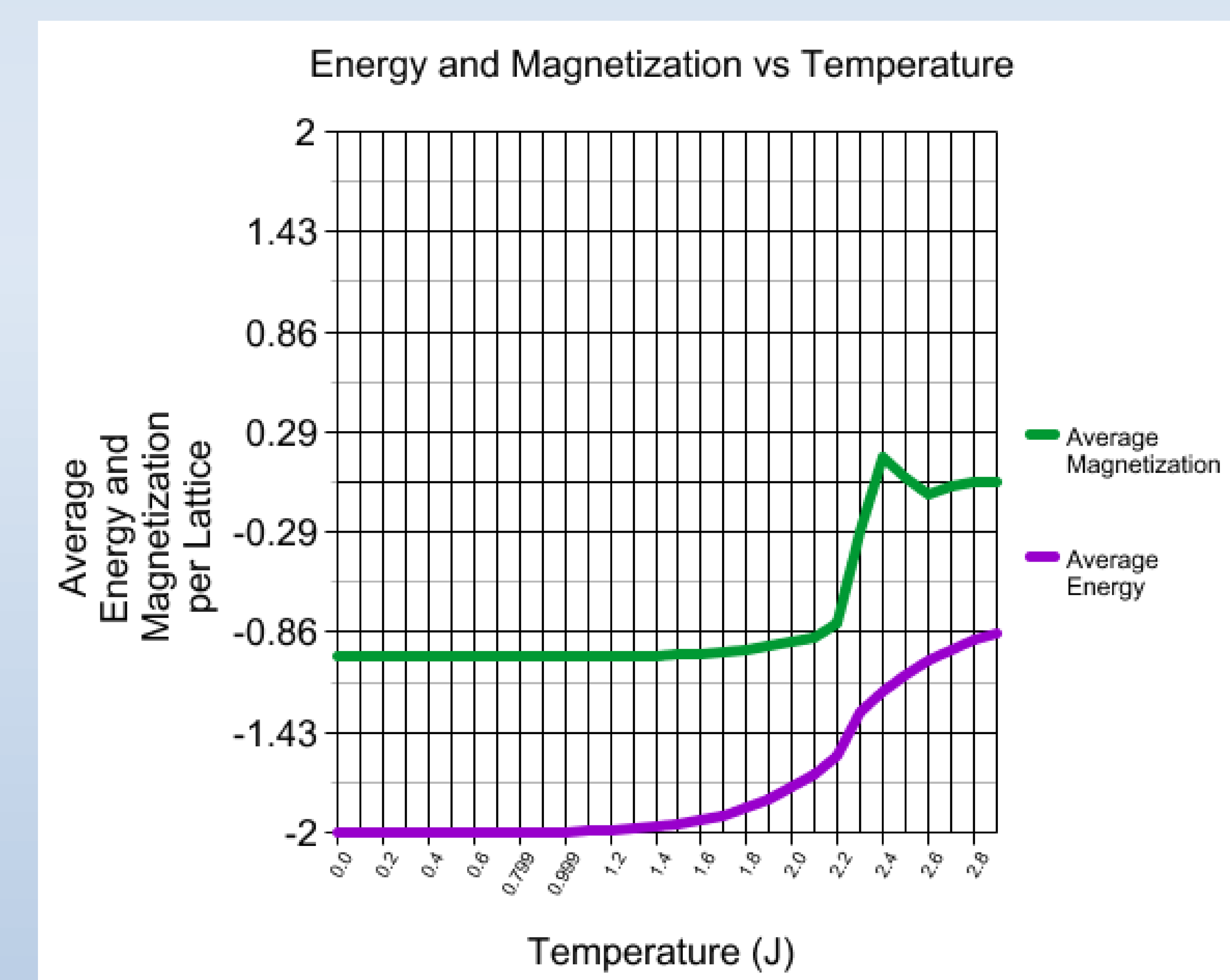
Temp = 2.49 J



Temp = 2.72 J

Analysis

- Blue square = Up spin
- White square = Down spin
- Simulation results show that T_c=2.27 J is the critical temperature, where the spins are approximately 50% up and 50% down
- $T<T_c$ → The system is usually either all down or up spins, or the net magnetization ≈ -1 or 1 respectively (ferromagnetic)
- $T>T_c$ → The spins are randomly aligned, approaching in a net magnetization ≈ 0 (paramagnetic)
- <E> increases as T increases
- As T approaches T_c → There is a sharp increase in energy



Acknowledgements

A special thank you for the help and support:

Dr. Ken D. Jordan, Ph. D.

Kevin Gasperich, Graduate Student

Kaye Archer, Graduate Student

Andrew L. Lotz, Ph. D.

Patrick Mullen, Director of Undergraduate Research

Kerry Lynn Soso, Office of Undergraduate Research