Potts Model:
Ising Model but Australian

By: Flor Nardone,
Carter Chapman,
& Dev Singh

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What is the *Potts Model?*

Ising vs Potts

Ising Model:
Statistical Model used to describe Magnetism. Takes a sum of interaction energies between a particle and its nearest neighbor. Limited to only **2 spin states**.

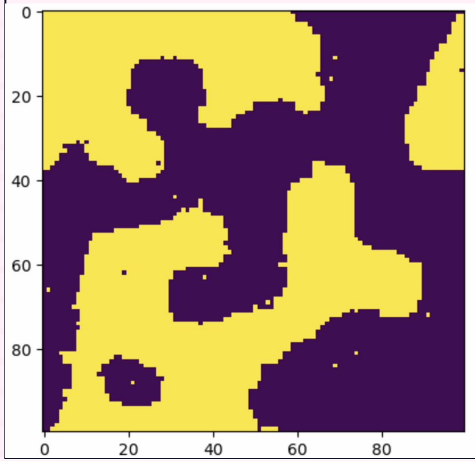
Potts Model:
Generalized version of **Ising Model**. Works on a system of **N spin states** (on image to right there are 3 spin states). Takes sum of interaction energies of nearest neighbors.

0	1	1
0	1	0
1	0	1

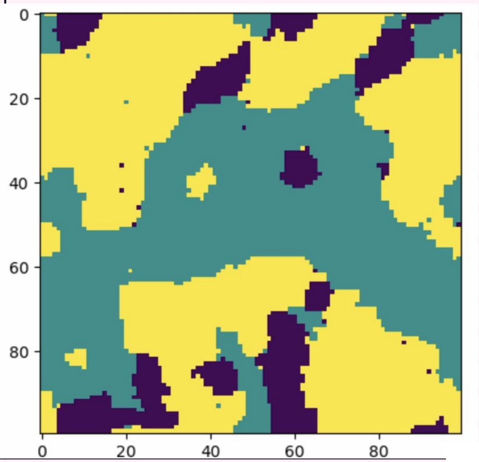
0	1	2
0	2	0
1	0	2

Note (for both):
- 100x100x100
- image taken during middle of simulation (described later on)

Isings Visual



Potts Visual



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Introduction

Applications:

- Magnetic Properties
  - We will discuss this in depth throughout the presentation
- Grain Growth
- Cellular Mechanosensing
  - Can predict dynamics of cell shapes
- Crystal Properties
  - Ex. behavior of atoms adsorbed on material surface (like graphene)
- And More!

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Math (quick recap)

$$h_1(\omega) = -J \sum_{\{i,j\} \in E(G)} \delta_{\sigma_i,\sigma_j}$$

- J = coupling constant,
  - determines how strong interactions between spins are
- $(\langle E^2 \rangle - \langle E \rangle^2)/\mathrm{Vol} = C_v$
- Calculates the Specific Heat of system

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Algorithm

- Propose spin flip
- Calculate the change in energy from changing spin
- If $\Delta E < 0$, then we keep the proposed spin
- If "**a**" (random number between [0,1]) < $e^{(-\beta*\Delta E)}$ then we keep proposed spin (Metropolis-Hastings)
- β is the inverse of temperature

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02

Simulations & Relationships

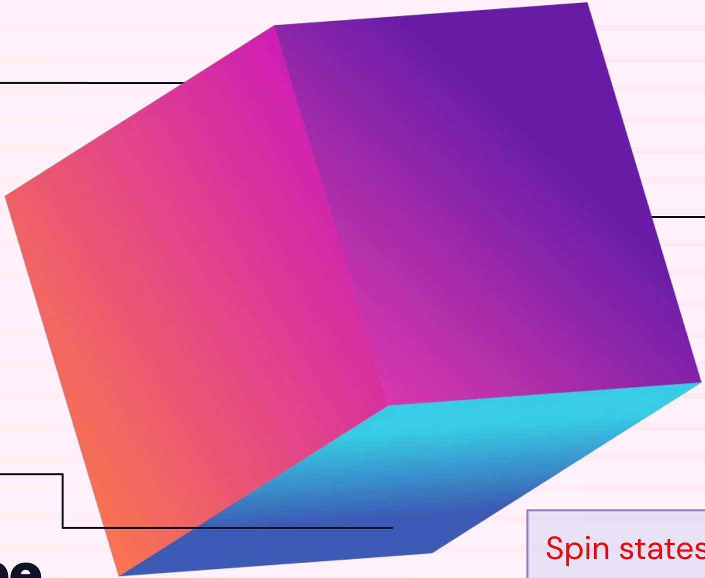
Python simulations for multispin lattices

About the cube:

Size

N x M x K

We did a variety of sizes such as 20x20x20



Lattice

Square/Cube

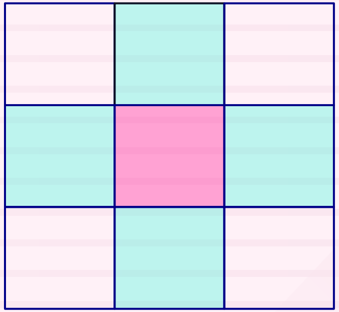
Our simulations were run on square (2D) and cube (3D) lattice.

Nearest Neighbors

6 nearest neighbors

Cube lattices have 6 nearest neighbors:

- Up
- Down
- Left
- Right
- Infront
- Behind



Spin states of the nearest neighbors as compared to the suggested spin state for the point of interest are used to calculate the Hamiltonian

- This is used in our Metropolis hastings algorithm as part of acceptance criteria
- Hamiltonian is saved and used to make Energy vs Time & Temperature vs Specific Heat Graphs

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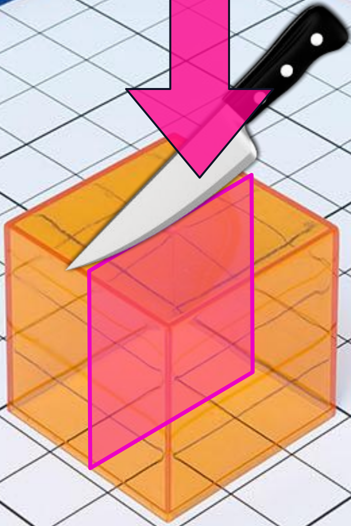
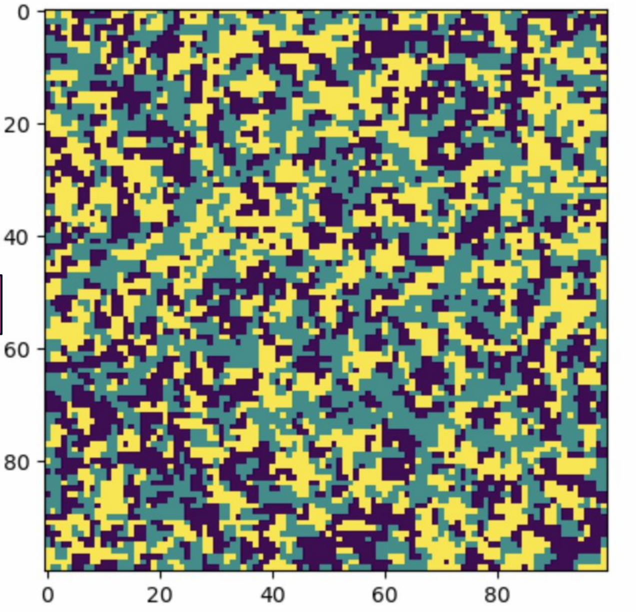
Our model:
The Cross Section

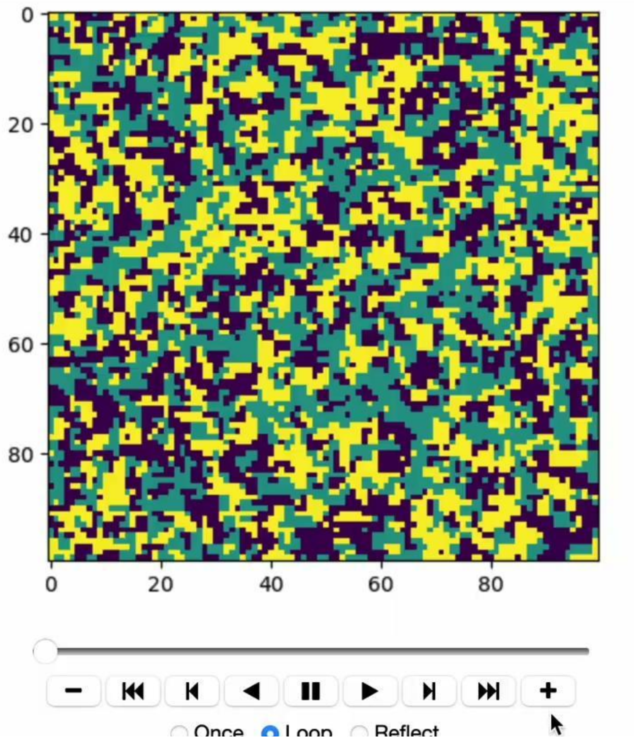




Initial State (t = 0)
- Randomized Spins (disordered)
- Size: 100x100x100
- Slice 50 of Kth dimension

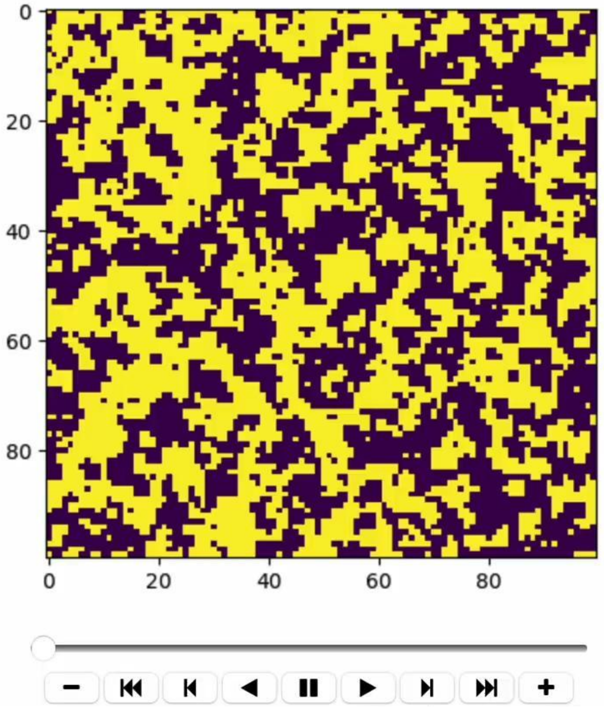
Running Cross Section

Potts Model (3 spins)



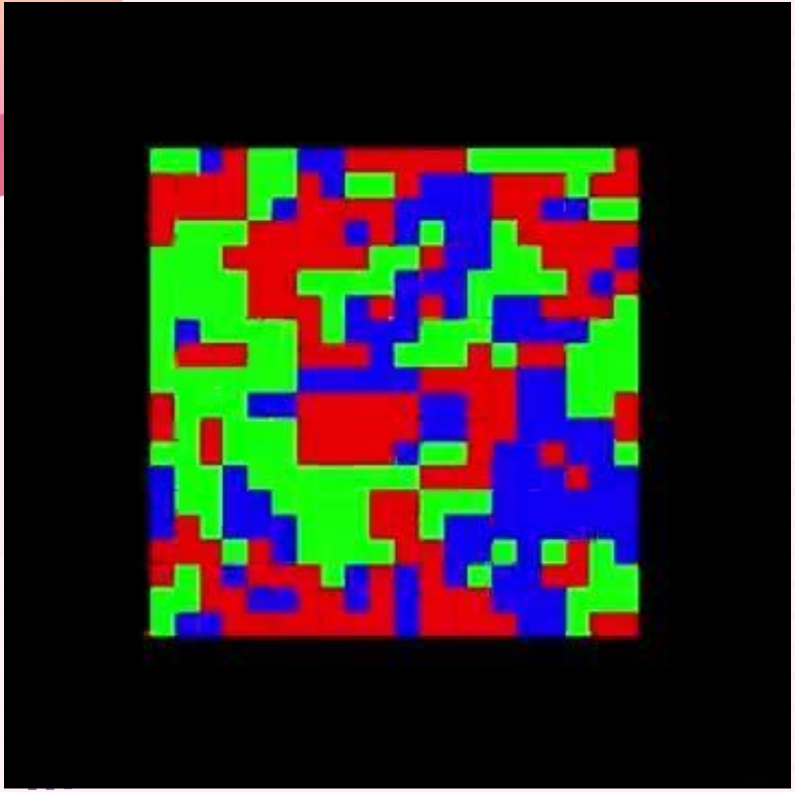
- Randomized Spins (disordered)
- B = 1.2

Isings Model (2 spins)



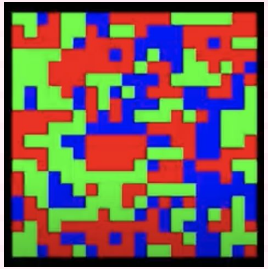
- Randomized Spins (disordered)
- B = 1.2

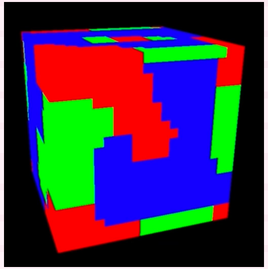
3D Simulation

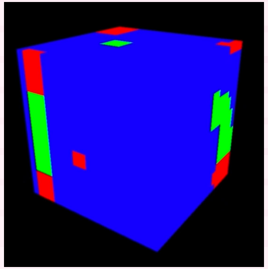


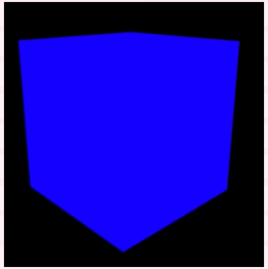
Using:
- Pygame
- PyOpenGl
- Pillow

Functions:
- 3D Potts Model visualization
- W, A, S, D rotation
- Runs over time
- Renders all faces









Limitation:
- trouble rendering for larger sized lattices
- Periodic Boundary Conditions (does not always perfectly approximate reality)

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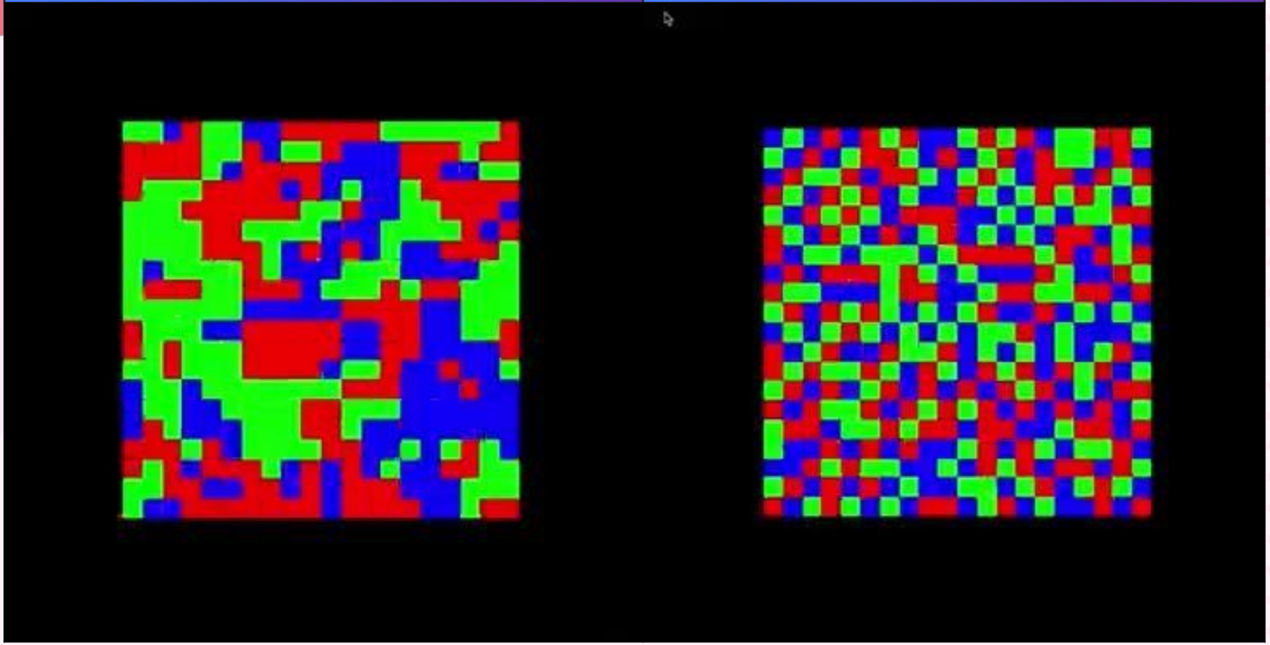
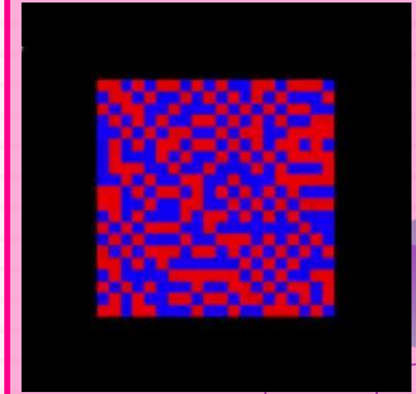
3D Simulation Cont.

Ferromagnetic J = + (positive)	**Anti-Ferromagnetic** J = – (negative)



Note (for both):
- B = 5
- 20x20x20
- Starting from disordered state

Note Isings Anti-Ferro:



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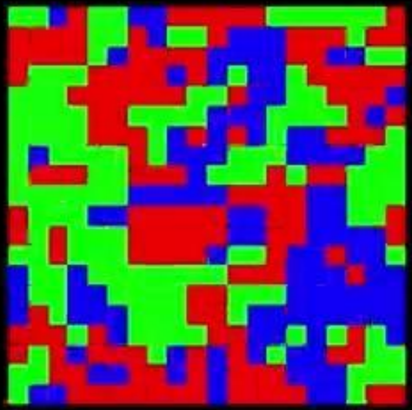
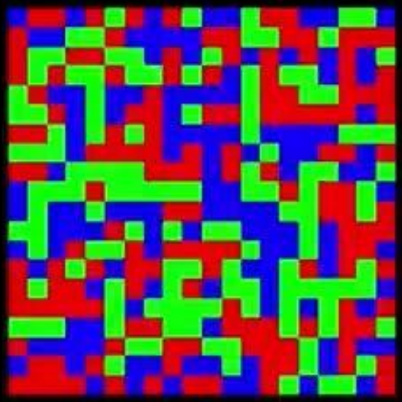
3D Simulation Cont.

Lower temp (Ferro) B = 5 (order)	Higher temp (Ferro) B = 0.1 (disorder)
	

Thermal Energy (Entropy) dominates

Interaction Energy dominates

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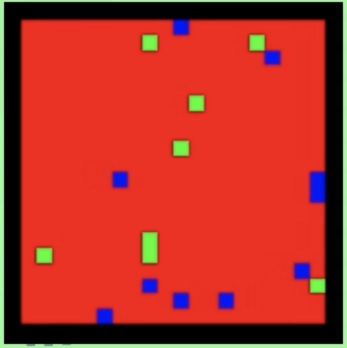
3D Simulation Cont.

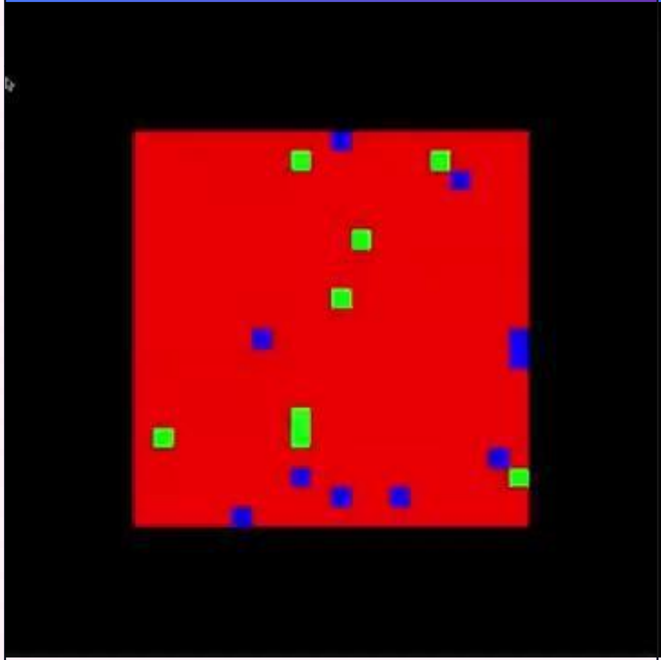
The **first frame** of the **ordered initial state** simulation looks like:



Order Initial State

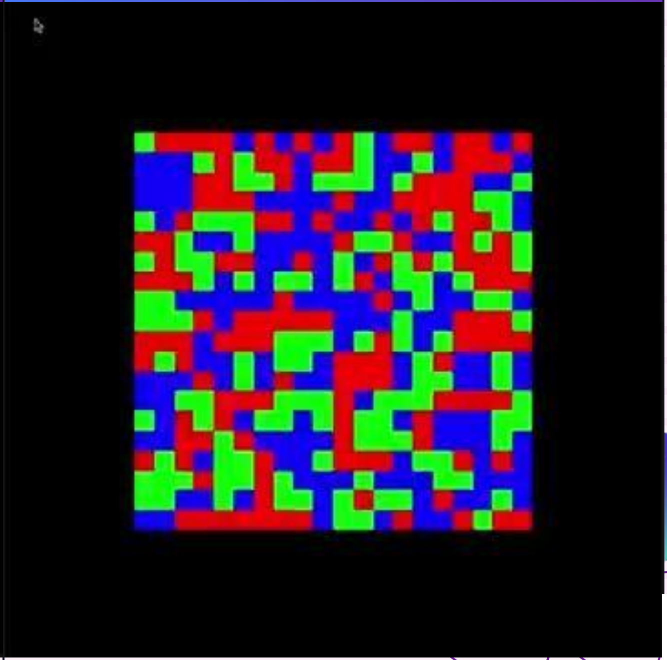
One spin in initial lattice

B = 0.5



Disordered Initial State

Randomized spin lattice



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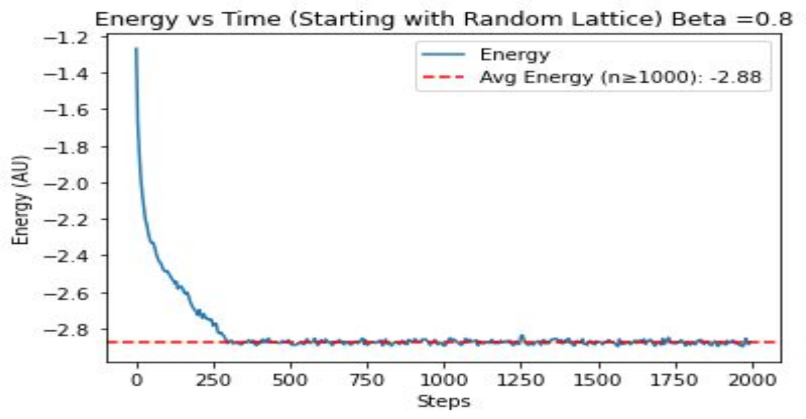
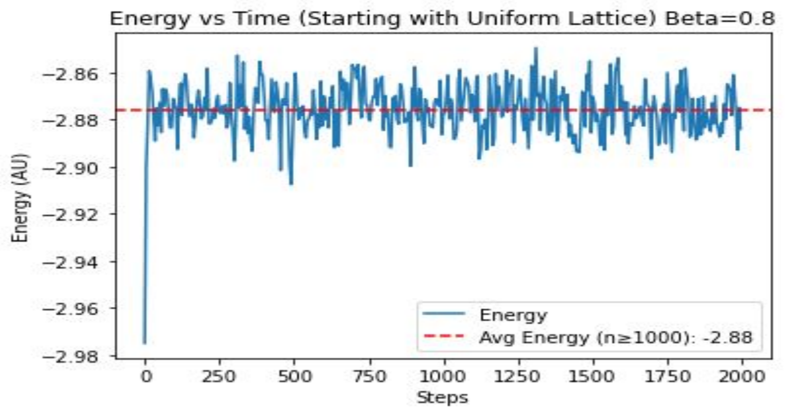
Graphs and Results

Energy vs Time
Temperature vs Specific Heat

Energy vs Time





Plots show the total lattice energy vs steps(time) in the algorithm. Different plots have a beta value associated.

Each beta value has two plots, one where the lattice is initially random and one where the lattice is initially uniform.

No matter what the initial state of the lattice is, the energy should converge to the same value over time as shown by the plots.

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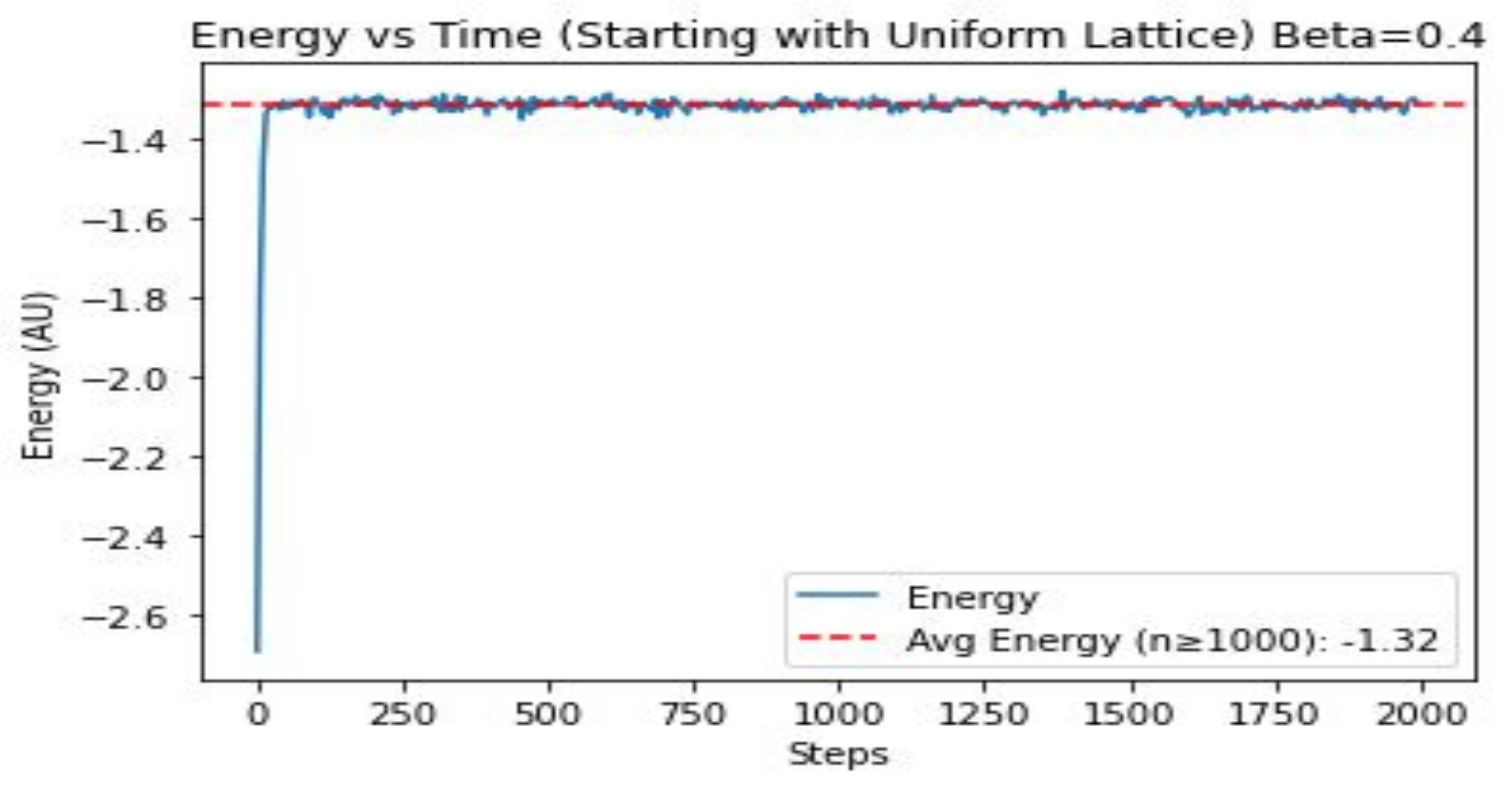
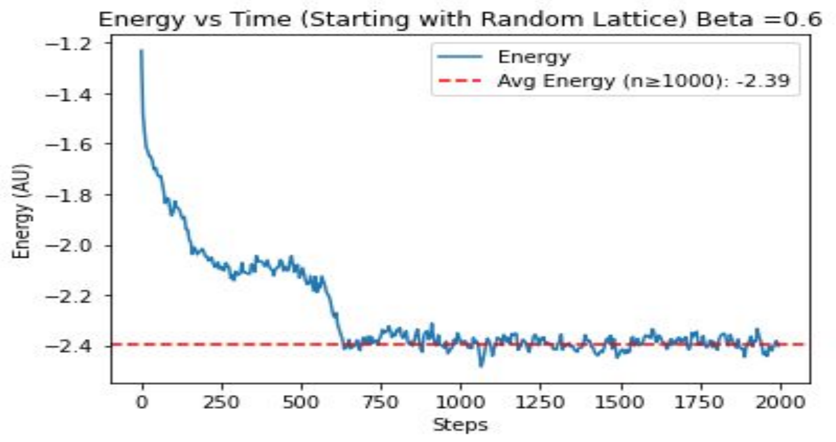
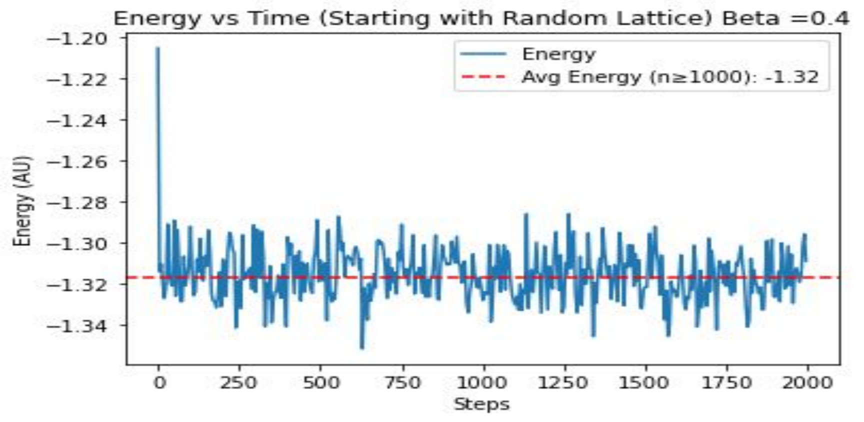
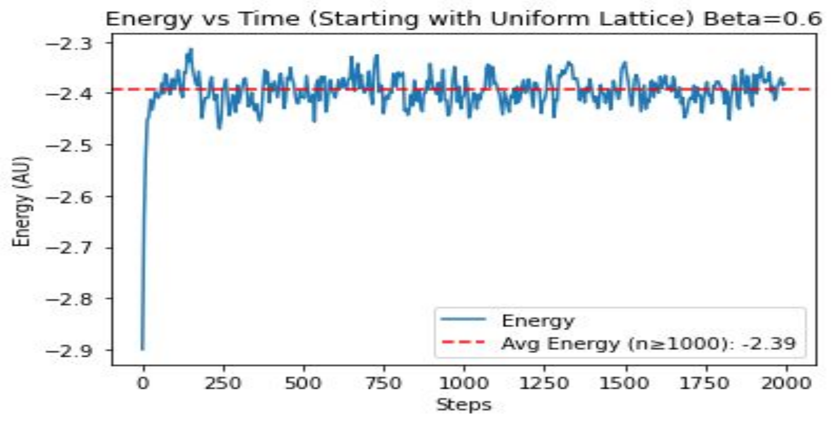
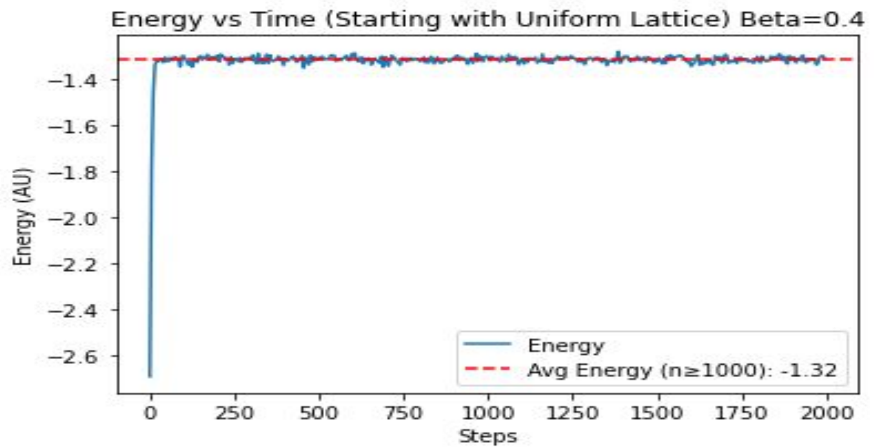

Energy vs Time (Starting with Uniform Lattice) Beta=0.4
Energy (AU)
−1.4
−1.6
−1.8
−2.0
−2.2
−2.4
−2.6
0
250
500
750
1000
1250
1500
1750
2000
Steps
Energy
Avg Energy (n≥1000): -1.32

Energy vs Time (continued)

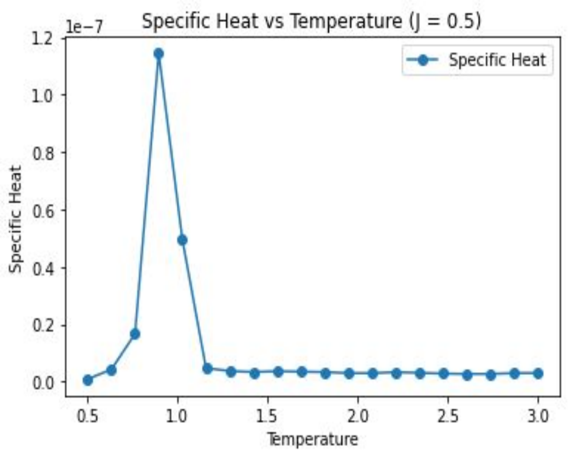


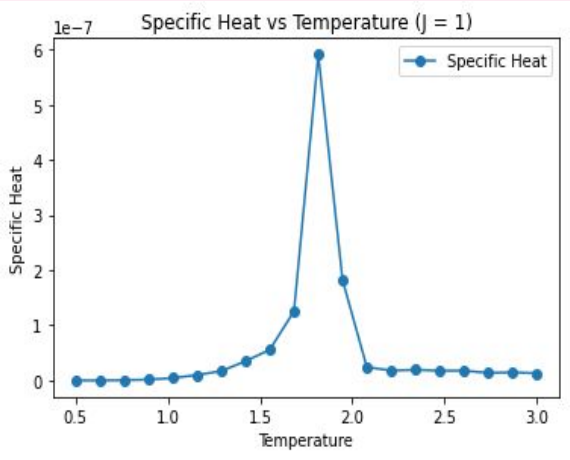


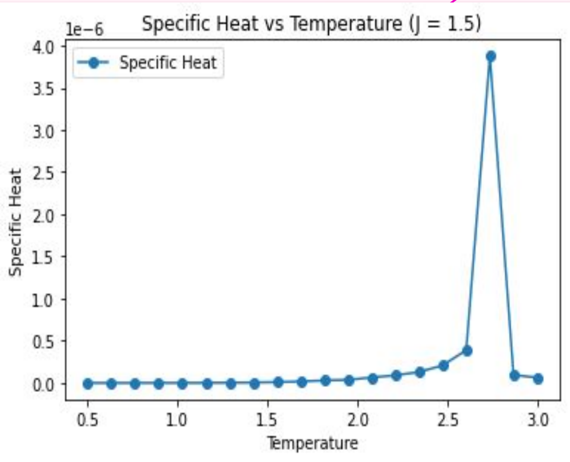


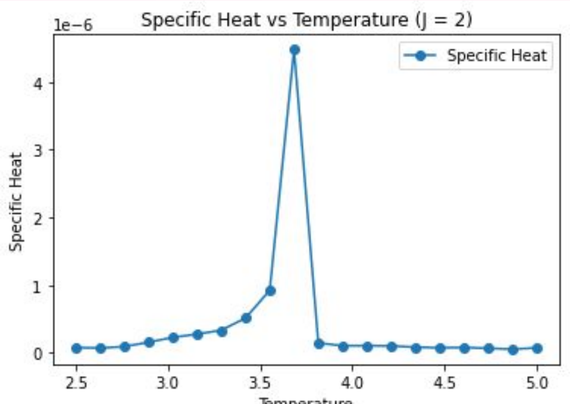


Temperature vs Specific Heat









Figures show the specific heat of a lattice compared with the temperature of the system. Different graphs show results for different coupling constants (J). Distinct peak indicates a phase transition of the system. As J increases so does the temperature where the phase transition occurs.

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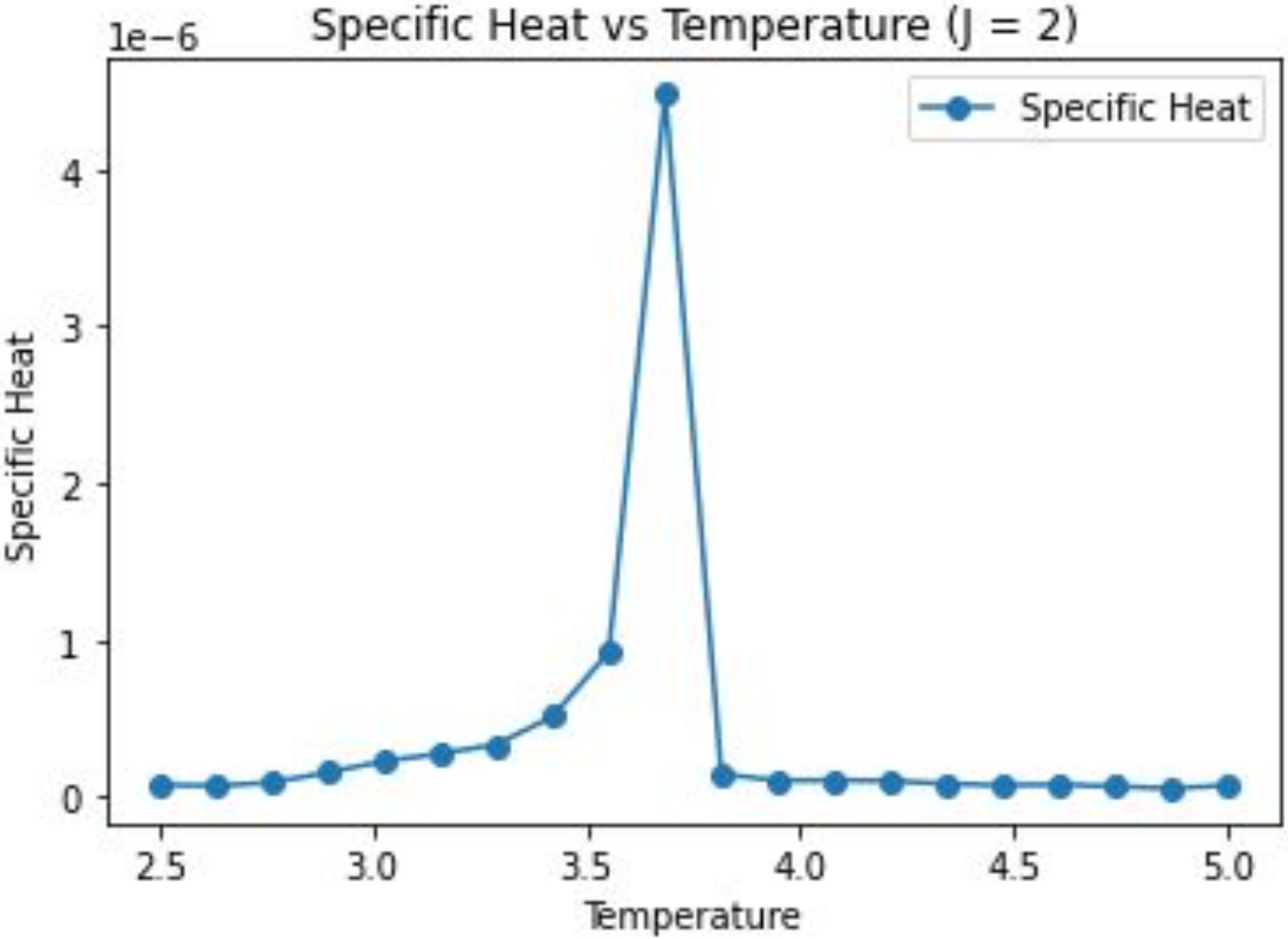
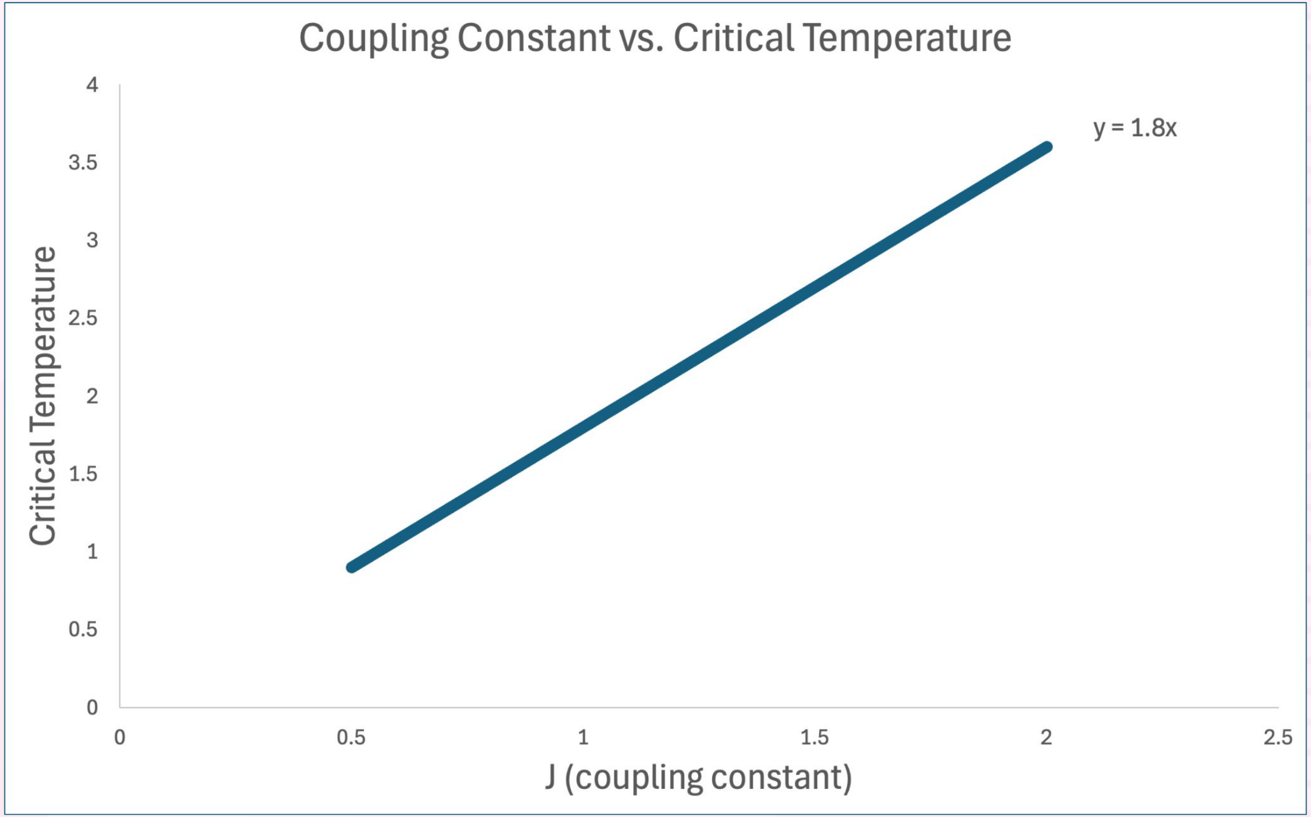

Specific Heat vs Temperature (J = 2)
1e−6
Specific Heat
Specific Heat
Temperature
0
1
2
3
4
2.5
3.0
3.5
4.0
4.5
5.0

Observation



- Relationship between the coupling constant and the critical temperature is linear!
- Slope is 1.8
- Small Sample size needs more investigating

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04

Outlook & The Future

Things we could change
Optimization

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Different types of lattices

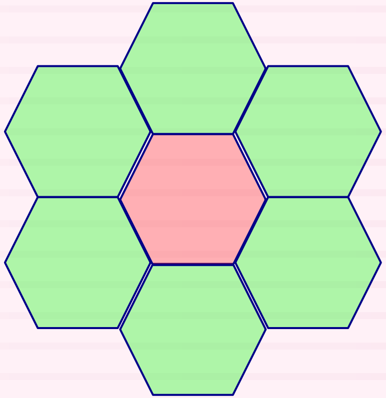
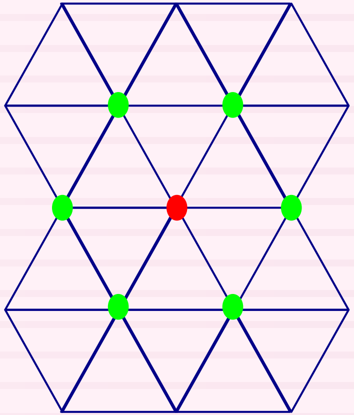
Using different types of lattices changes the nearest neighbors and thus the Hamiltonian. Lattice geometry is what defines the connectivity of the spin states and thus changing it can drastically change the properties.

Honeycomb:

- In 2D has 6 nearest neighbors
- The association between one data point and another can be more precise due to more short-range neighbors
- Can be more computationally intensive
- Ex) Carbon atoms are arranged in a honeycomb (graphene)

Triangular:

- Usually also has 6 nearest neighbors because it is commonly defined differently
    - Note: if that same definition was used for a square lattice it would have 8 nearest neighbors

Honeycomb	Triangular
	

Other Improvements

Optimization

- Different ways to propose spin changes
- Changing groups of spins at a time for faster convergence, Ex. Swendsen Wang Dynamics or spin clusters

Relationships

- More research on the relationship between the Critical Temperature and coupling constant
- How does the number of states affect critical temp.
- Lattice size and critical temp.

Applications

- Use model to simulate different scenarios such as protein mutations in biology
- Use potts model to minimize noise in a signal

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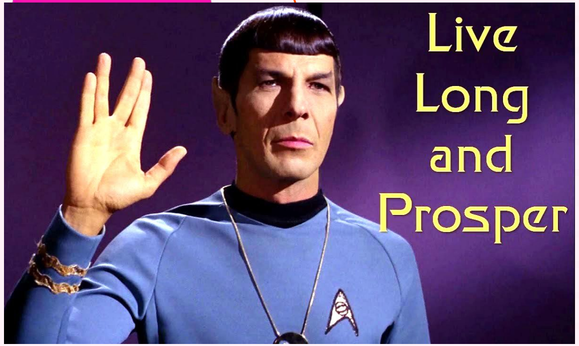
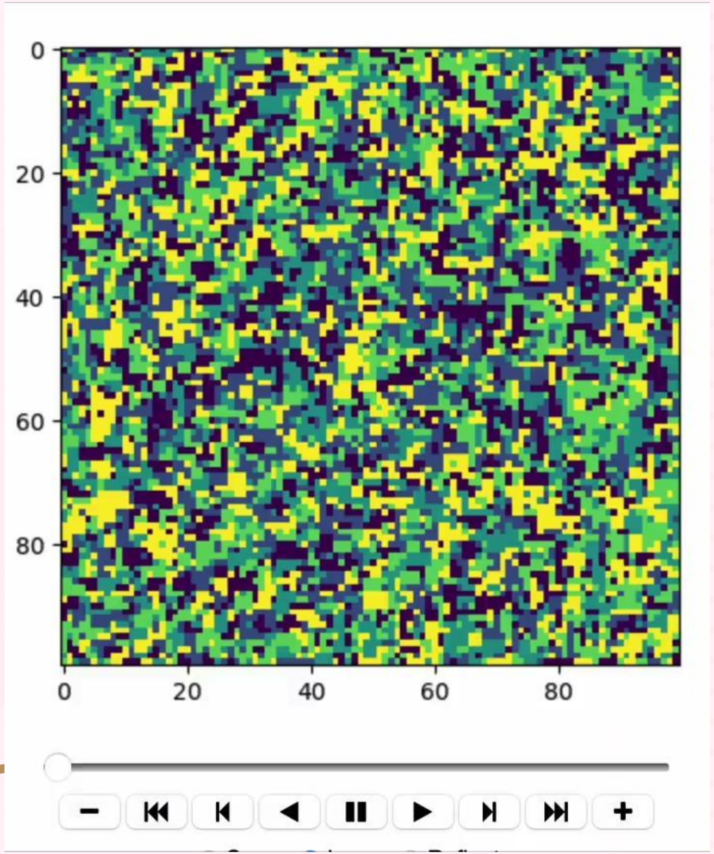


The End

Questions?

Extra Slide: Cross Section with more spins



Note:
- 5 spin states
- J = 1
- B = 1.2

Extra Slide: Answers to possible questions

Why not use diagonal nearest neighbors?

This is a convention.

The goal of the Potts model (as well as the Isings model) is to test the effects of short-range interactions. The strongest interactions occur between spins that are in close proximity. Diagonal nearest neighbors are further away and generally interact more weakly.

What are the units?

The units are arbitrary.

What about Paramagnetism?

The common version of the Potts Model does not account for Paramagnetism. To do so we would have to add a variable that accounts for the application of an external magnetic field.

Extra Slide: Answers to possible questions

Does it have to run on Metropolis Hastings?

No.
There are other models that can simulate the Potts Model such as:

- Glauber Dynamics,
- Swendsen-Wang Dynamics

What if J is a decimal instead of just +1 and -1?

This just represents a weaker ferromagnet/antiferromagnet.

For example if J = 0.5 then it is still tends to ferromagnetism but it is not considered a “hard ferromagnet.” Likewise, a coupling constant of -0.2 (J = -0.2) is considered a weak antiferromagnet.

What are the Boundary Conditions?

We are using Periodic Boundary conditions. This essentially means that the edges wrap around eliminating edge effects. We do this so that every spin has a full set of nearest neighbors.

Extra Slide: Cool Stuff

Link to Cool Isings Model Simulation:

- https://visualize-it.github.io/ising_model/simulation.html
- You can change the temperature, coupling constant (interaction strength), updates per iteration, & grid size

Sources

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