Numerical Simulation of the 2D Ising Model Using the Metropolis Algorithm

A powerful technique in statistical mechanics for understanding phase transitions in ferromagnetic materials.

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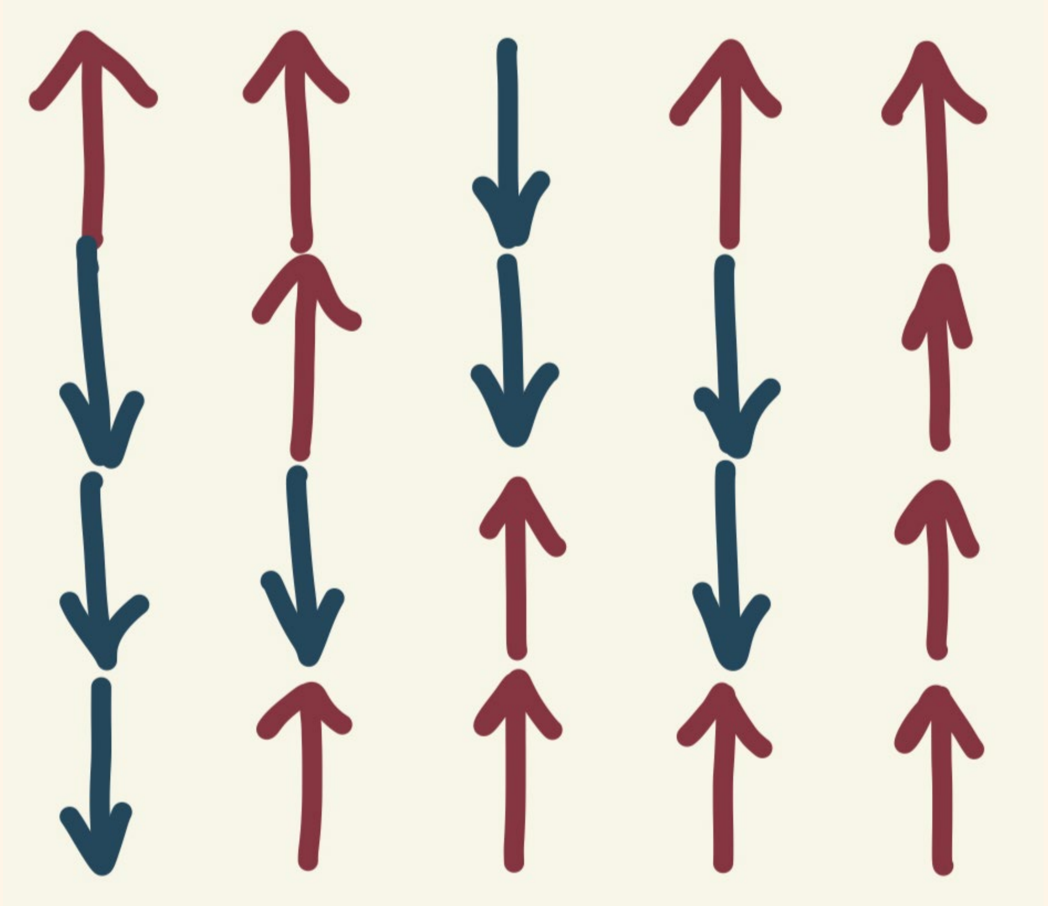
Introduction – The Ising Model

- Developed by Ernst Ising in 1925
- The Ising model is a mathematical model used in statistical mechanics to study **ferromagnetic** materials.
- It consists of an n x n lattice of particles, represented by spins ($S_i \pm 1$), that **interact with their nearest neighbors**.
- Describes **phase transitions** from ferromagnetism (ordered) to paramagnetism (disordered).
- The phase transition occurs at a **critical temperature, $\boldsymbol{T_c}$**, where $T_c = 2.269 \ldots \mathrm{J/K_b}$. The system is ordered when $T < T_c$ and disordered when $T > T_c$.



Ferromagnetism occurs when electron spins spontaneously align parallel to each other, creating a net magnetic moment below a critical temperature. For example, Iron is ferromagnetic below 1043K (770°C), meaning it maintains a magnetic moment even in the absence of an external magnetic field, which is why it can be used to make permanent magnets and is attracted to magnetic fields.

Introduction – Statistical Mechanics

Statistical Mechanics utilizes a powerful probability function for systems in thermodynamic equilibrium via the partition function:

Partition Function

$$Z = \sum_i e^{-\beta E_i}$$

Probability Function

$$P_\mu = \frac{1}{Z} e^{-\beta E_\mu}$$

This probability is known as the Boltzmann distribution, where $\beta = 1/k_B T$. It shows that:

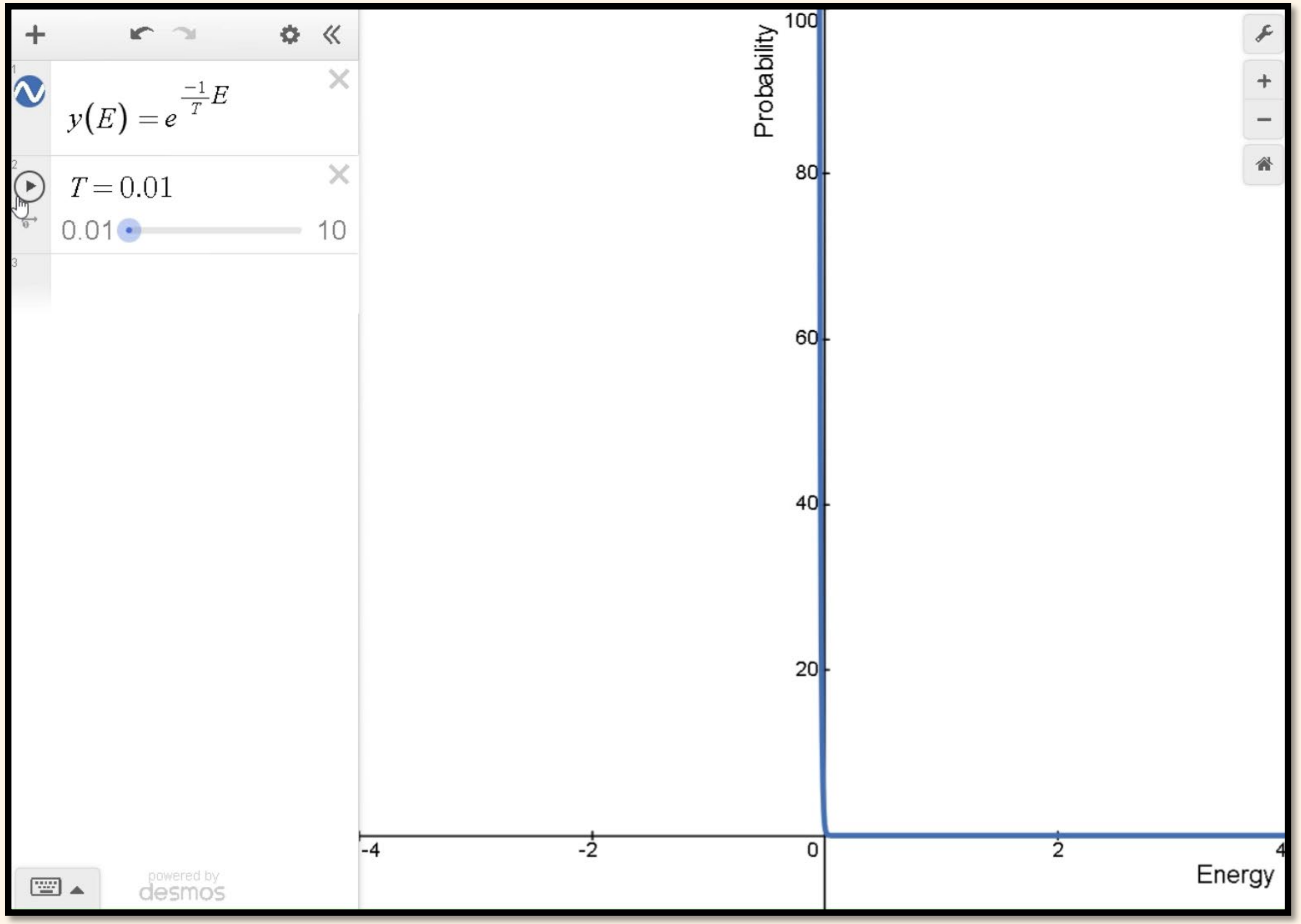
- States with lower energy are exponentially more likely than states with higher energy
- As temperature increases (β decreases), the exponential term becomes less steep, making the probability distribution more uniform

Another fundamental principle in statistical mechanics and stochastic processes is the **detailed balance principle:**

Detailed Balance

$$p_i P(i \rightarrow j) = p_j P(j \rightarrow i)$$

This principle will be used to enforce that the simulation converges to the correct equilibrium distribution


$y(E) = e^{\frac{-1}{T}E}$
$T = 0.01$
0.01
10
Probability
100
80
60
40
20
-4
-2
0
2
4
Energy
powered by
desmos

Our goal is to simulate the **2D Ising mode**l using the **Metropolis-Hastings algorithm** to observe the **phase transitions** that occur at the **critical temperature**.

By plotting magnetization versus temperature and validating against known analytical solutions, we aim to demonstrate how a ferromagnetic material loses its magnetic properties above the critical temperature Tc, while showing convergence to theoretical predictions as the lattice size increases.

Metropolis-Hastings Algorithm

A Monte-Carlo Simulation

The algorithm finds the equilibrium state in the magnet at a particular temperature. We initialize with a random distribution of spin up and spin down particles (represented with a +1 or -1), and iterate over the system:

1. Get the current state of the lattice, E_i
2. Pick a random particle on the lattice and flip the spin sign, E_j. Calculate the change in energy induced by this sign change, $\Delta E = E_j - E_i$. We want to find the probability that the system will accept this new state and update the system accordingly.
   - If $\Delta E < 0, P(i \to j) = 1$. The flip is favored and the sign change is accepted.
   - If $\Delta E \geq 0, P(i \to j) = e^{-\beta \Delta E}$. The change will be accepted based on the probability from the detailed balance principle.
3. Repeat n^2times per step to $\approx$ update each particle once

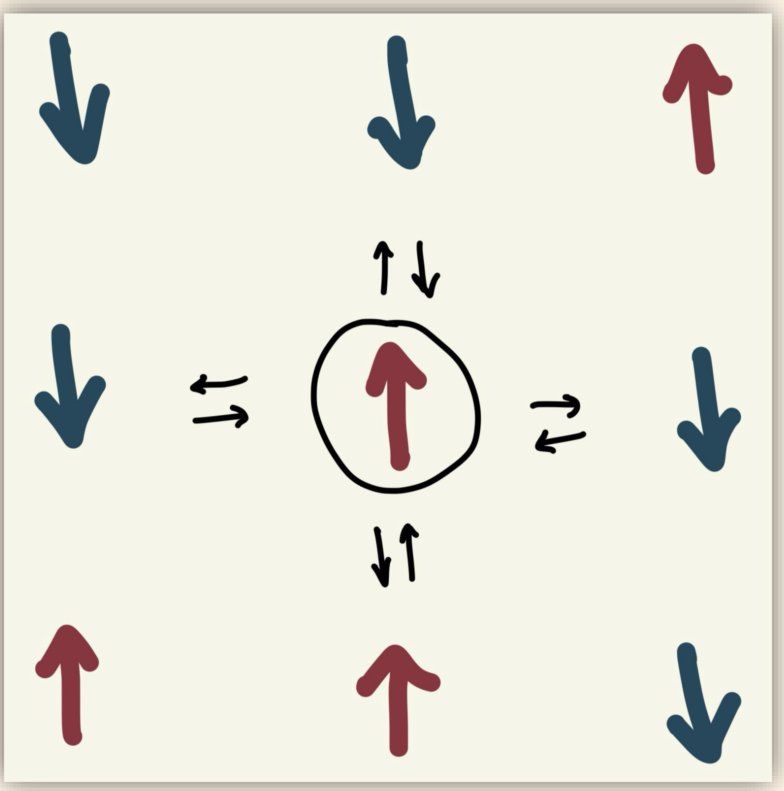
Energy Equation

$$E_\mu = -J \sum_{<i,j>} S_i S_j - hS_i$$

ΔE Equation

$$\Delta \mathrm{E} = 2JS_i \sum_{<i,j>} S_j - hS_i$$

Example



$$\Delta E_i = 2J s_i \sum_{\langle i,j \rangle} s_j + h s_i \quad , \quad J = 1, h = 0$$

$$= 2 s_i \sum_{\langle i,j \rangle} s_j = 2S_i \left(S_{i+\hat{x}} + S_{i-\hat{x}} + S_{i+\hat{y}} + S_{i-\hat{y}} \right)$$

$$= 2(-1 - 1 - 1 + 1)$$

$$= 2(-2) = -4$$

The negative value indicates that the flipped spin moves the system to a lower energy level and thus is favorable.

ΔE Equation

$$\Delta E = 2JS_i \sum_{<i,j>} S_j$$

Implementation Details/Edge Cases

1 Boundary conditions

To handle the boundary spins, periodic boundaries are used using modulo/if-else statements

```
@njit
def compute_neighbors(spins, n, i, j):
    """Compute sum of neighboring spins with periodic boundary conditions."""
    return (spins[(i+1) % n, j] + spins[(i-1) % n, j] +
            spins[i, (j+1) % n] + spins[i, (j-1) % n])
```

2 Monte Carlo Update Rule

This is the heart of the Metropolis algorithm. We decide whether to flip the spin based on the energy change and the current temperature.

```
@njit
def metropolis_step(spins, J, T, n):
    """Perform one Metropolis update step for the system."""
    for _ in range(n ** 2):  # Attempt to flip each spin once on average
        i, j = np.random.randint(0, n, size=2)
        deltaE = compute_delta_energy(spins, J, i, j, n)
        if deltaE <= 0 or np.random.rand() < np.exp(-deltaE / T):
            spins[i, j] *= -1
```

3 Finite-Size Scaling Analysis

This problem bridges the gap between the finite simulation and theoretical predictions for infinite systems, highlighting the impacts of simulation size.

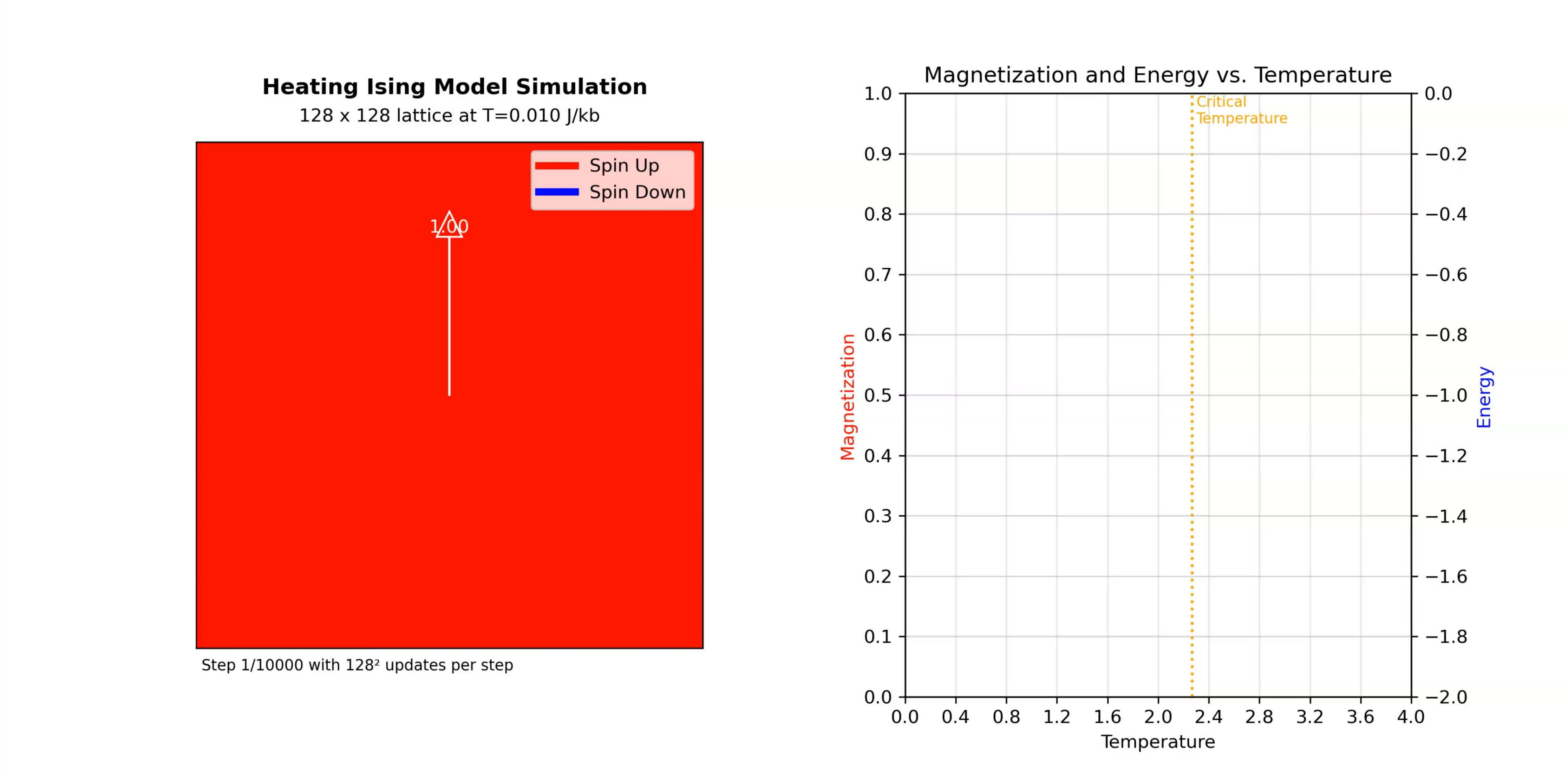
- The lager the lattice, the more closely the simulation will mimic theoretical predictions of T_c. However, the simulation will be more computationally expensive.
- Typically, one would want to find a good trade-off between accuracy and speed.
- Using periodic boundaries helps to mitigate the effects of this problem, but as we will see in the results, there is still an impact on the apparent critical temperature

4 Testing

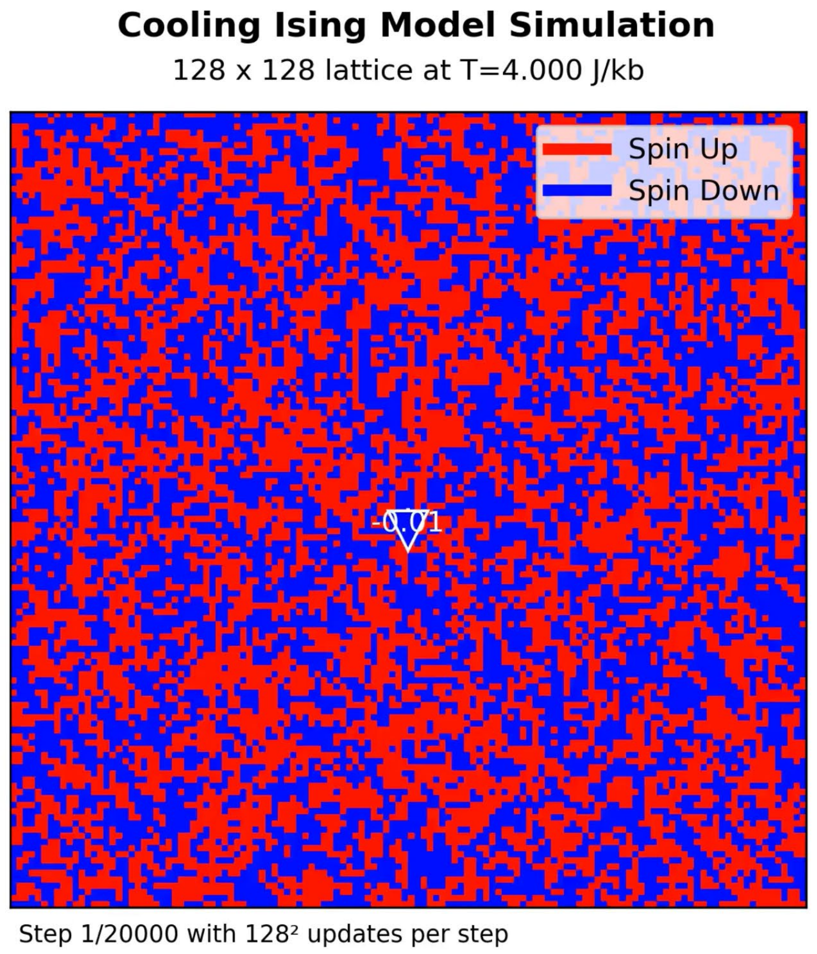
Based on the resulting graph, we know if the simulation is performing as expected if:

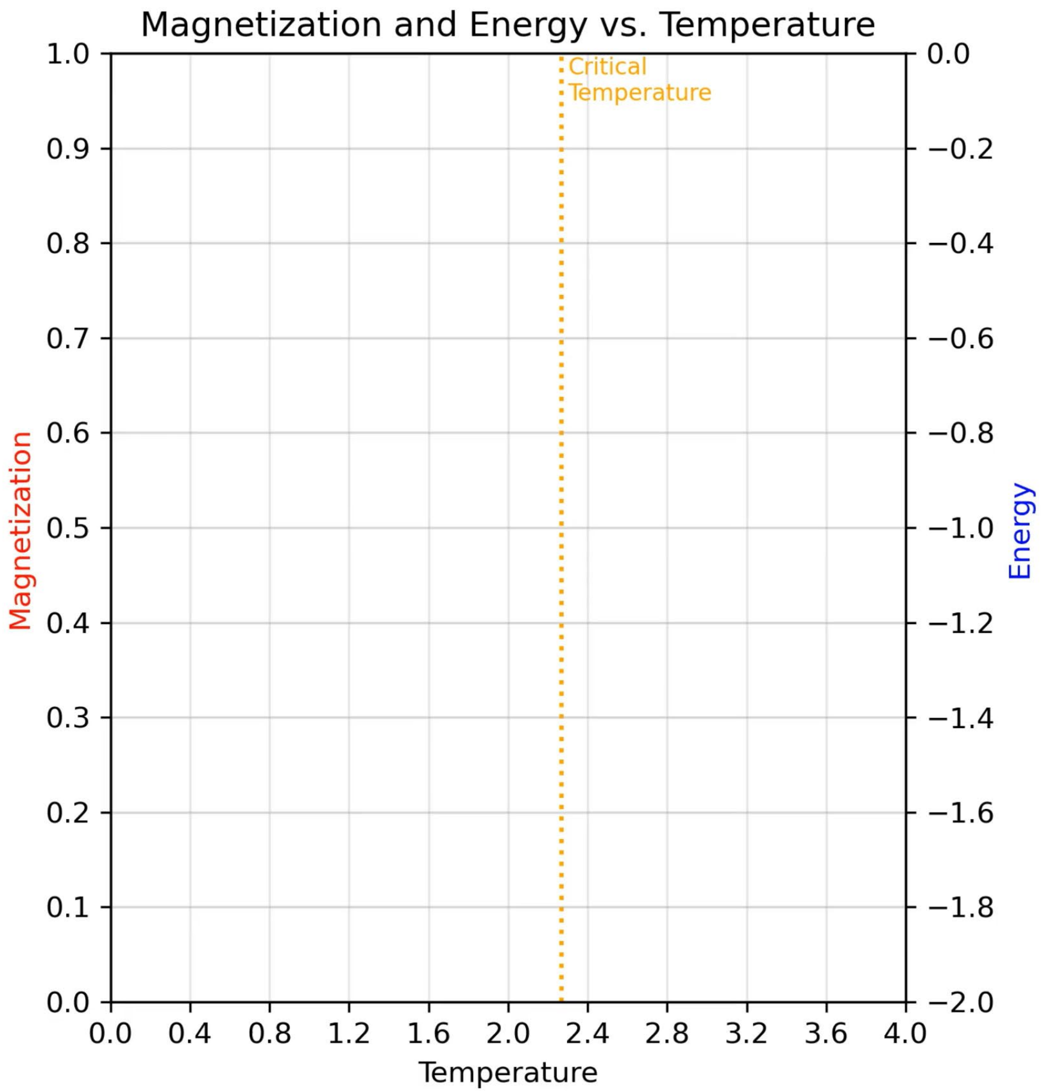
- Magnetization is ≈ 1 when $T < T_c$
- Magnetization is ≈ 0 when $T > T_c$
- Magnetization transitions from 1 to 0 around the known T_c

Results - Observing Phase Transitions

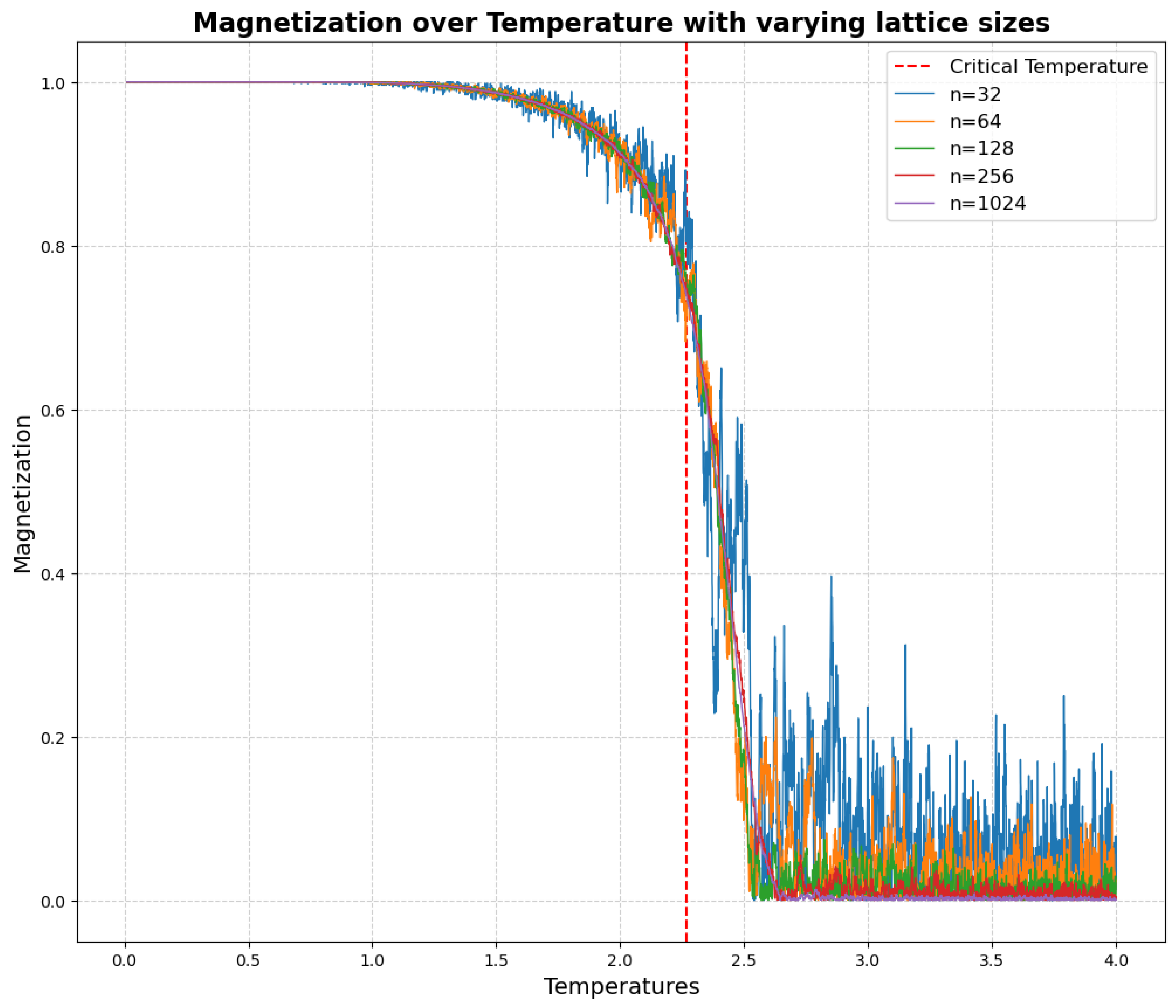


Results - Observing Phase Transitions





Results – Finite-Scaling Results



Conclusion

Main Goals:

1. **Critical Temperature Verification** – Successfully observed phase transition in the 2D Ising model with the estimated T_c converging around the known exact solution of $2.269\ J/K_b$.
2. **Finite-Size Scaling** – Demonstrated proper scaling behavior with system size, showing the effects on accuracy.

Other accomplishments:

- **Computational Performance-** Achieved significant speedup through Numba optimization, enabling simulations of larger lattices in reasonable timeframes.
- **Visualization-** Created dynamic visualizations of the phase transition, showing how magnetization and energy values are affected in real-time.