

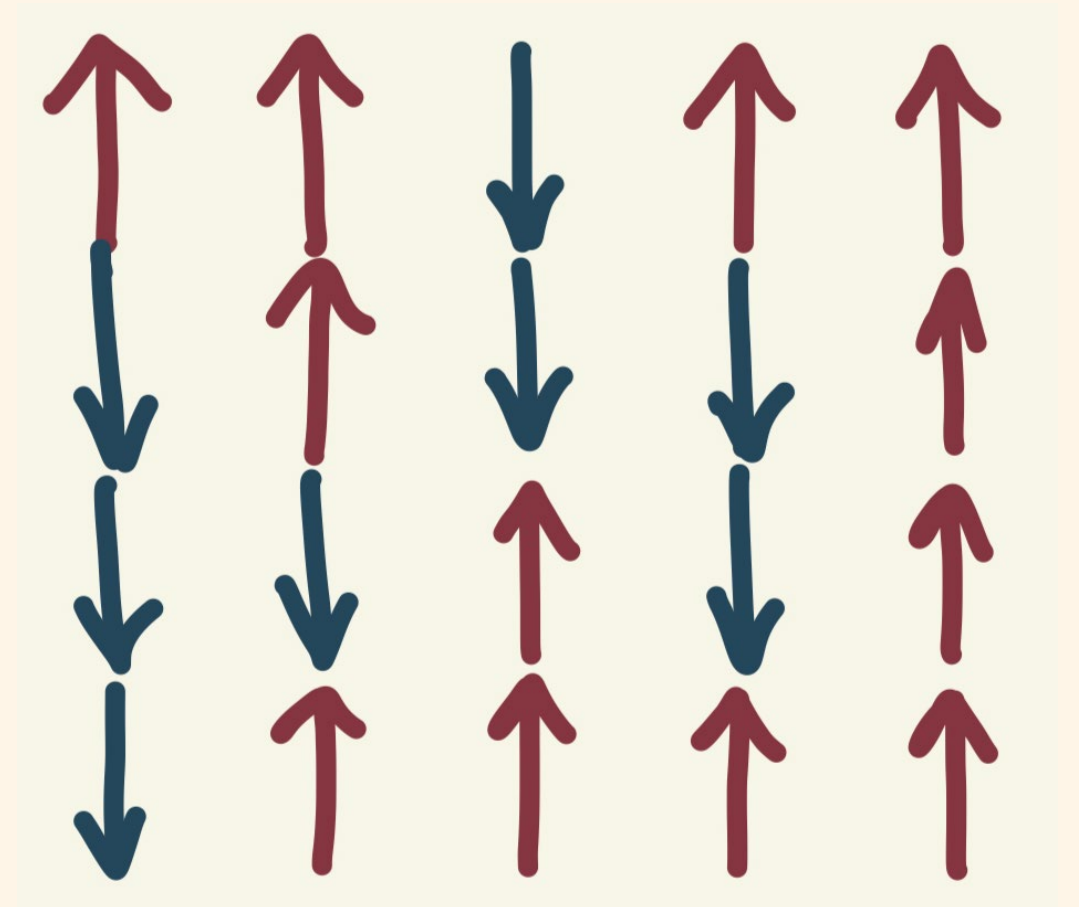
# Numerical Simulation of the 2D Ising Model Using the Metropolis Algorithm

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

**Isabelle Byrne**

# 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  $n \times n$  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,  $T_c$** , where  $T_c = 2.269 \dots J/K_b$ . 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:

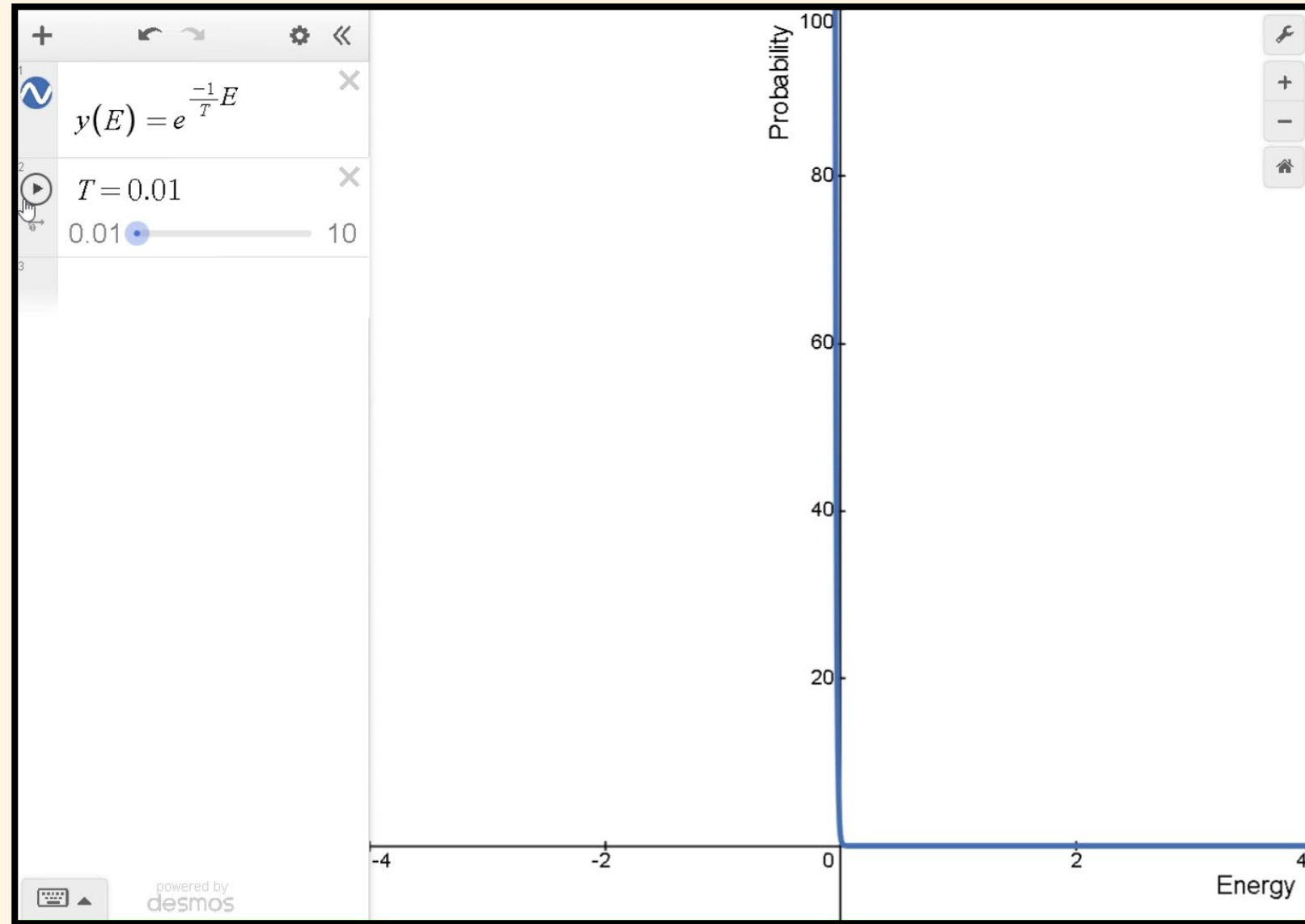
- States with lower energy are exponentially more likely than states with higher energy
- As temperature increases ( $\beta$  decreases), the exponential term becomes less steep, making the probability distribution more uniform

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



**Our goal** is to simulate the **2D Ising model** 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  $T_c$ , 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  $\Delta E < 0$ ,  $P(i \rightarrow j) = 1$ . The flip is favored and the sign change is accepted.
  - If  $\Delta E \geq 0$ ,  $P(i \rightarrow j) = e^{-\beta \Delta E}$ . The change will be accepted based on the probability from the detailed balance principle.
3. Repeat  $n^2$  times per step to  $\approx$  update each particle once

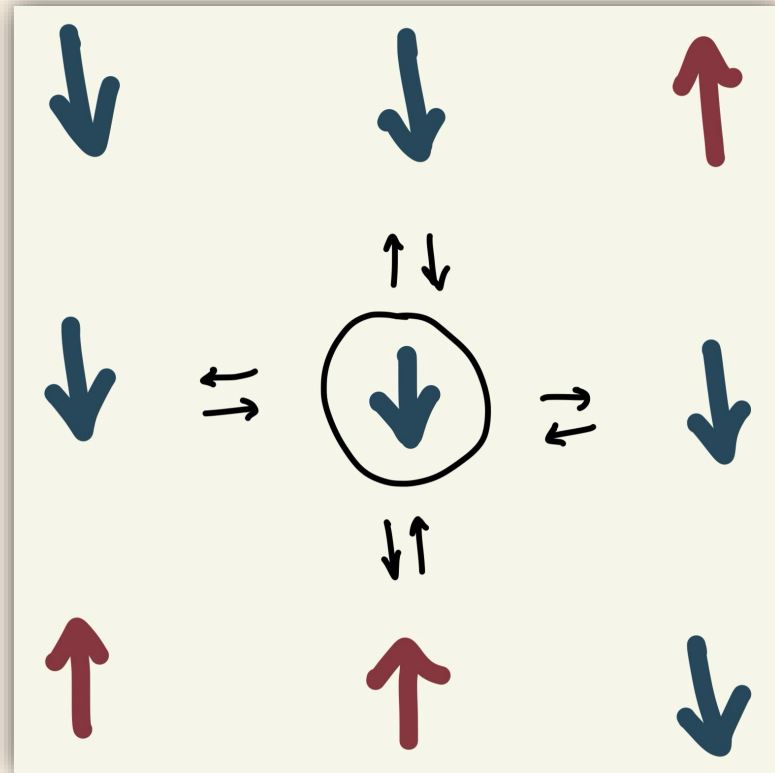
## Energy Equation

$$E_{\mu} = -J \sum_{\langle i,j \rangle} S_i S_j - h S_i$$

## $\Delta E$ Equation

$$\Delta E = 2J S_i \sum_{\langle i,j \rangle} S_j - h S_i$$

# Example



$\Delta E$  Equation

$$\Delta E = 2JS_i \sum_{\langle i,j \rangle} S_j$$

$$\begin{aligned} \Delta E_i &= 2J S_i \sum_{\langle i,j \rangle} S_j + h S_i, \quad J=1, h=0 \\ &= 2S_i \sum_{\langle i,j \rangle} S_j = 2S_i (S_{i+\hat{x}} + S_{i-\hat{x}} + S_{i+\hat{y}} + S_{i-\hat{y}}) \\ &= 2(-1 - 1 - 1 + 1) \\ &= 2(-2) = -4 \end{aligned}$$

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

# 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])
```

## 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 larger 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

## 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
```

## 4 Testing

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

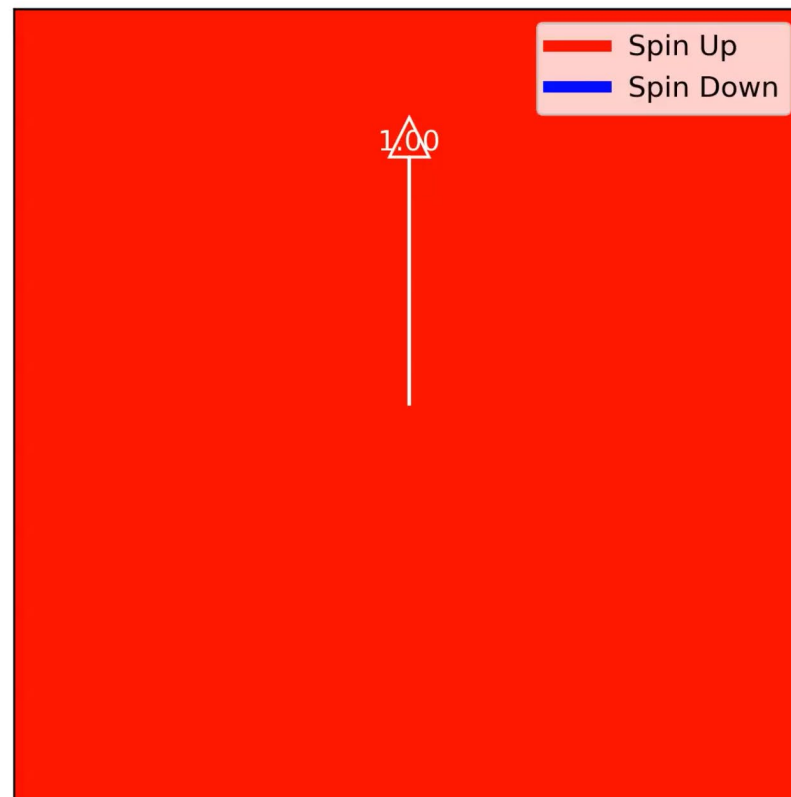
- Magnetization is  $\approx 1$  when  $T < T_c$
- Magnetization is  $\approx 0$  when  $T > T_c$
- Magnetization transitions from 1 to 0 around the known  $T_c$



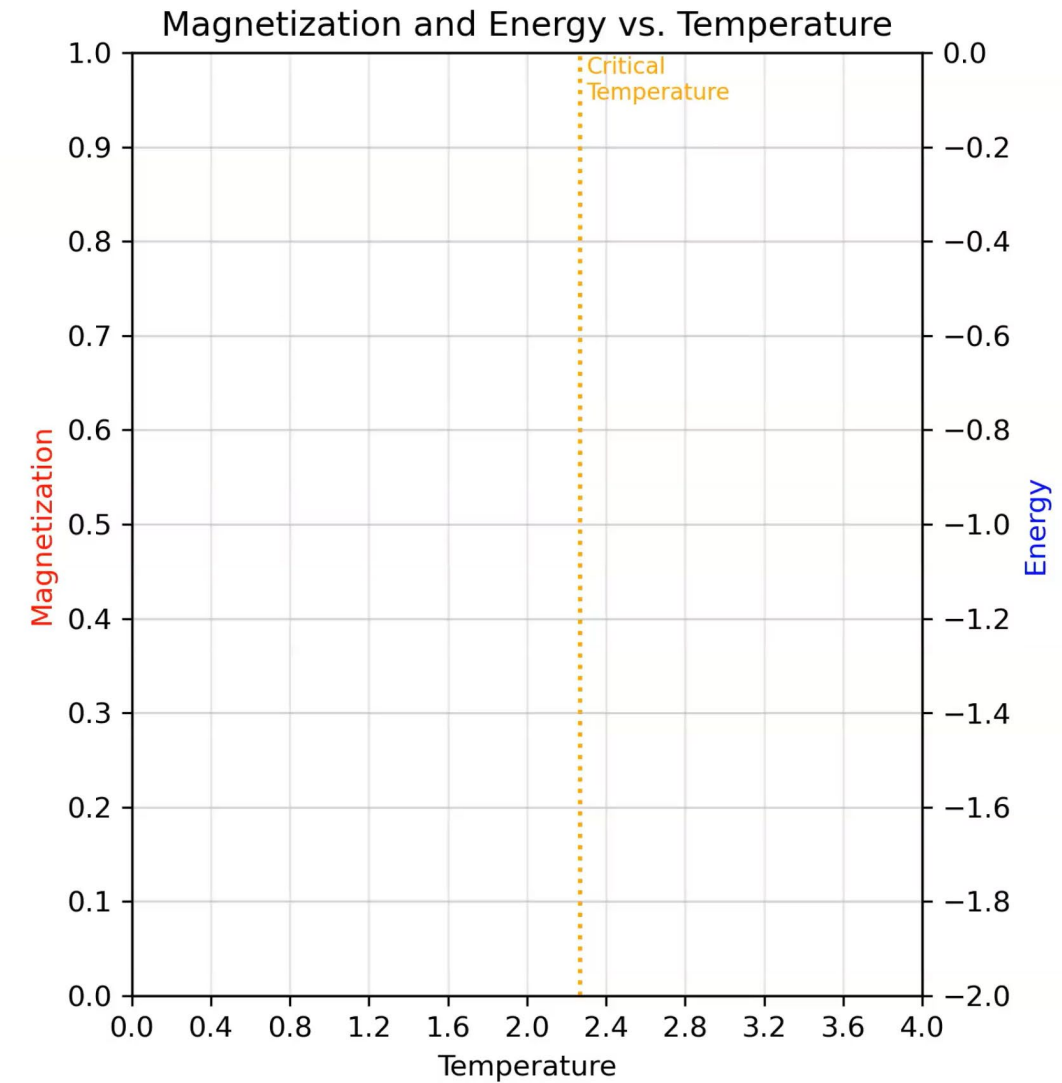
# Results - Observing Phase Transitions

## Heating Ising Model Simulation

128 x 128 lattice at  $T=0.010$  J/kb



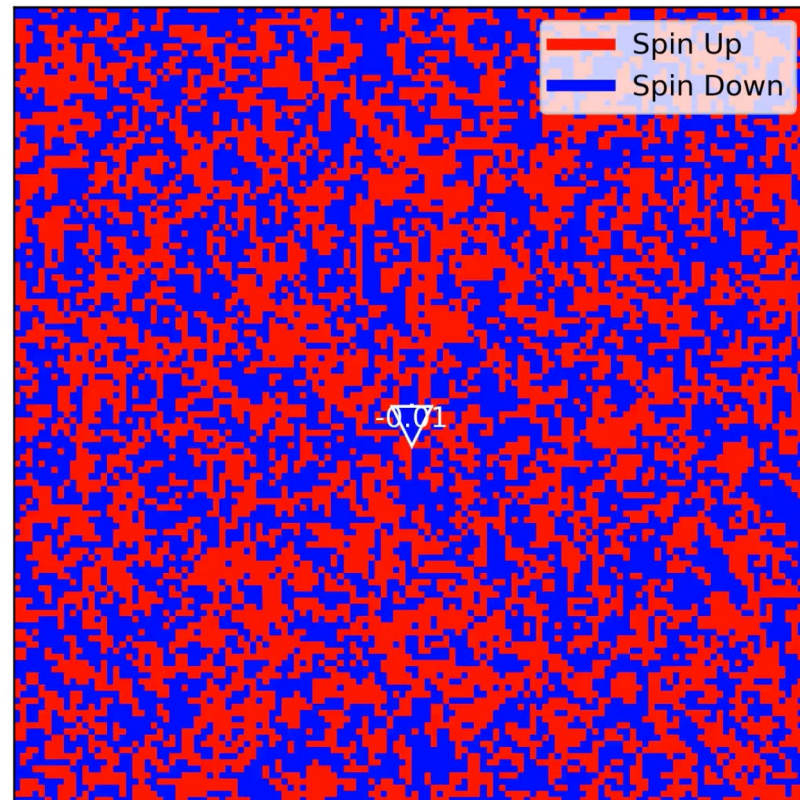
Step 1/10000 with  $128^2$  updates per step



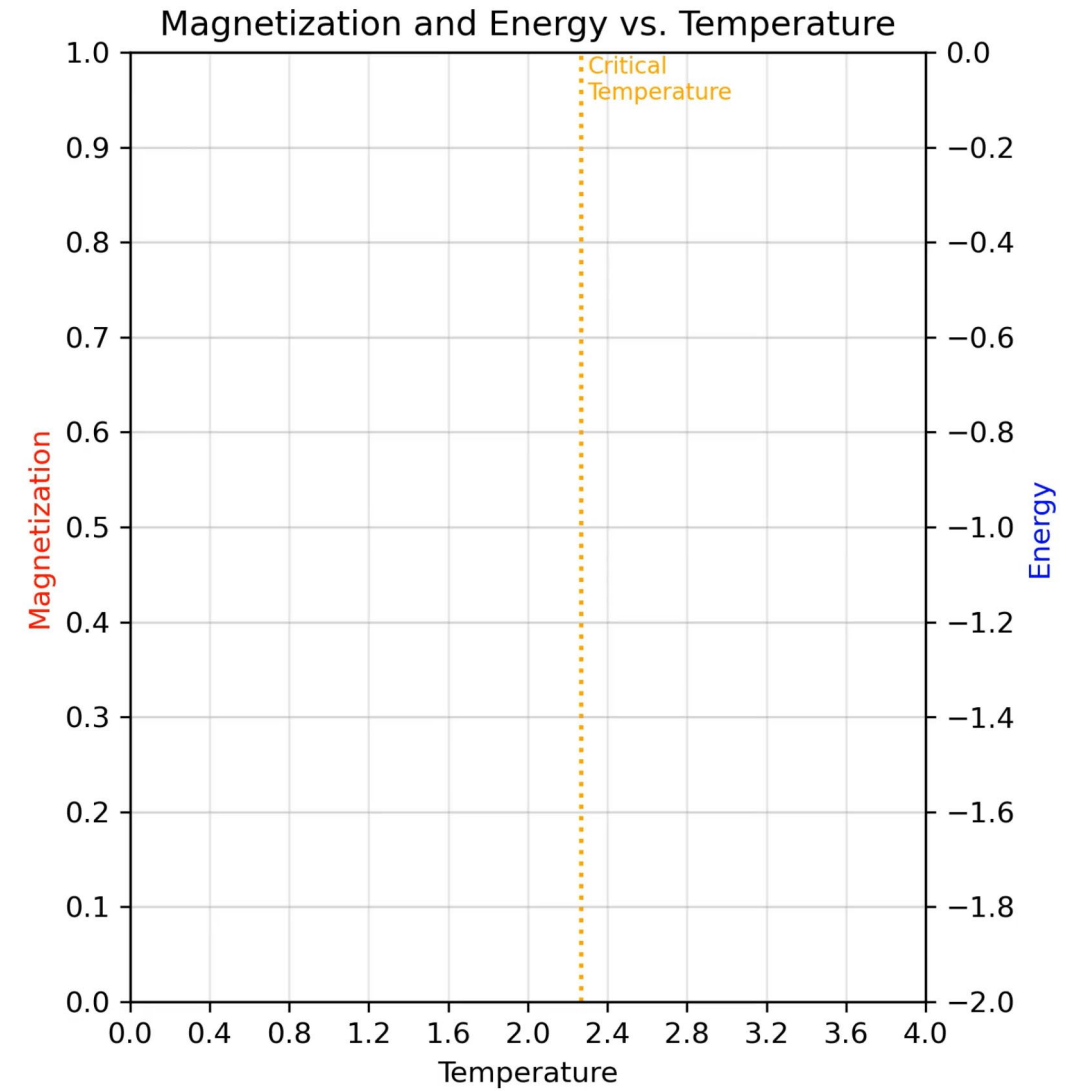
# Results - Observing Phase Transitions

## Cooling Ising Model Simulation

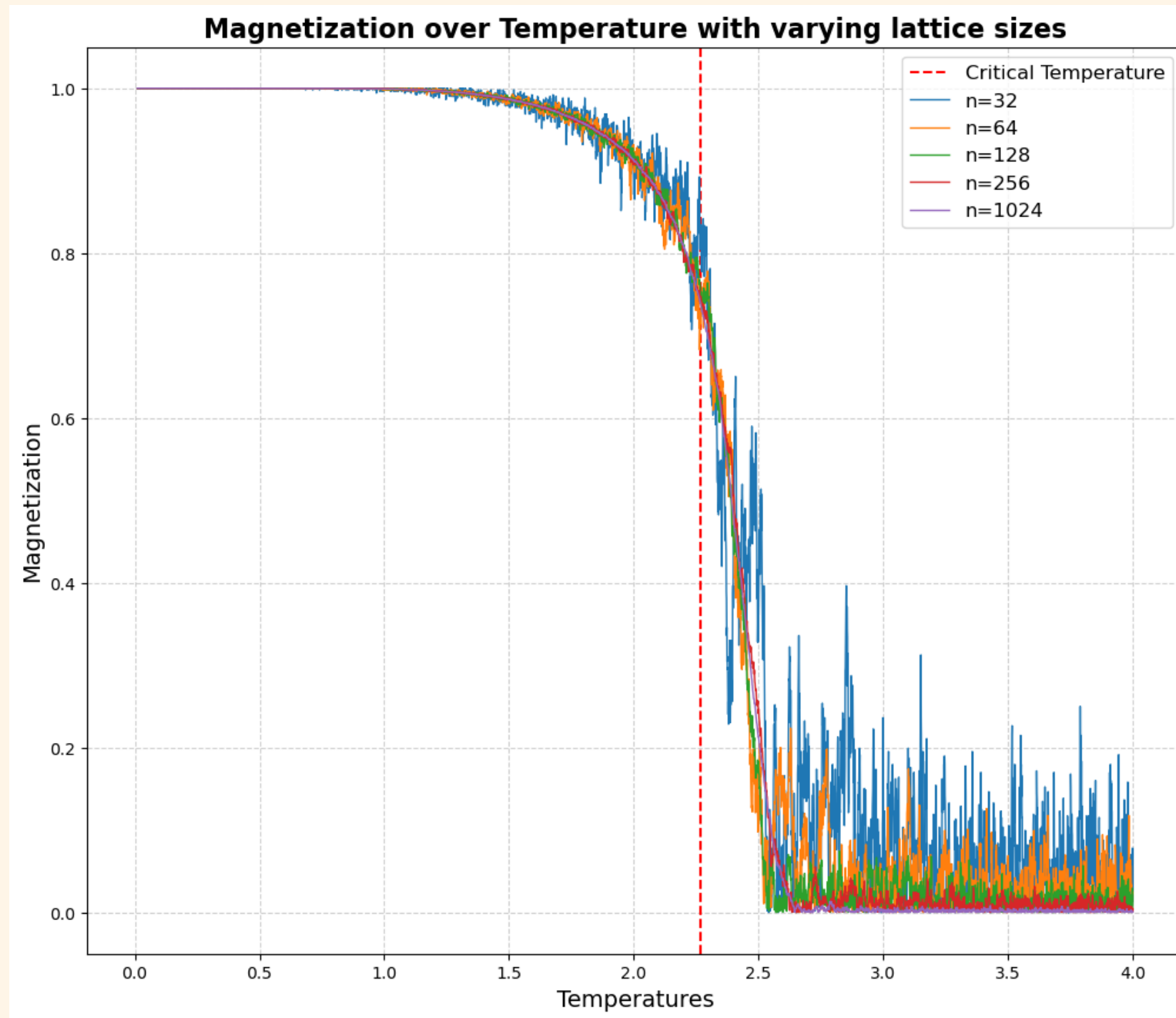
128 x 128 lattice at  $T=4.000$  J/kb



Step 1/20000 with  $128^2$  updates per step



# 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.