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Simulating Phase Transitions in Biological Systems Using the 2D Ising Model: A Statistical Physics Approach

Zachary Gao Sun[1], Vishva Kalaivanan[2]

Yale University

Abstract: ***This paper investigates how the Ising model, a foundational construct in statistical physics, can be employed to simulate phase transitions observed in biological systems such as protein folding and lipid membrane dynamics. Using the two-dimensional version of the model and the Metropolis-Hastings algorithm, the study explores binary state systems and analyzes temperature-dependent behaviors like spin clustering and energy variations. The findings demonstrate how these simulations mirror biological processes, offering valuable insights into mechanisms like molecular misfolding and cellular organization. This approach bridges theoretical physics with biological complexity, suggesting broader applications in fields such as neuroscience and genetic regulation.***

Keywords: Ising model, phase transition, biological systems, protein folding, Monte Carlo simulation

1. Introduction

Many biological processes, such as protein folding, cell membrane dynamics, and gene expression, exhibit characteristics similar to phase transitions observed in physical systems. By mapping the interactions within biological systems onto the Ising model, scientists gain deeper insights into the mechanisms of phase transitions and phase separations, which are necessary for understanding the fundamental processes that sustain life. This study aims to simulate and analyze biological phase transitions using the two-dimensional Ising model, with a focus on understanding temperature-driven behaviors in systems such as protein folding and lipid membrane organization.

The Ising model is a simple model that can be used to describe phase transitions and cooperative critical phenomena [4]. The Ising model on a two-dimensional square lattice, without a magnetic field, was analytically solved by Lars Onsager. While the Ising model was introduced to study phase transitions in ferromagnetic materials, it has found application in various scientific domains, including the analysis of biological systems. The partition function of the Ising model contains details about the states of the system and the probability of transitioning from one to the other. In our study, we use the 2d Ising model to study a 2-state system, namely, the ↑ state and the ↓ state, as a simplification for any arbitrary two-state systems that can exhibit phase separation.

Here, we use the Ising model, which is extensively used in statistical mechanics to model first and second-order phase transitions. For the Ising model, we have the partition function, defined as:

$$Z = \sum e^{-\beta H}$$

In which β is the Boltzmann constant (we unify β to be 1 throughout the simulation), and H is the Hamiltonian of the system.

The Metropolis-Hastings algorithm is a technique within Markov chain Monte Carlo (MCMC) that is used to generate a series of random samples from a probability distribution that is challenging to sample directly from. Additional samples are included in the sequence by following a two-step process: initially, a new sample is suggested utilizing the previous one, and then the suggested sample is either incorporated into the sequence or disregarded based on the probability distribution at that particular point. The sequence that is generated can be utilized for approximating the distribution, such as creating a histogram, or for calculating an integral.[1] The Metropolis algorithm is an algorithm that samples configurations of the Ising model at a given temperature. It starts off by picking a random single spin from the random configuration of spins on the lattice and calculates the change in energy (delta energy) when flipping the spin. If $\Delta E \leq 0$, the spin is flipped. This algorithm is used in Phase transitions, Magnetization, and Specific heat.[2]

The Ising model has been applied in various fields since its introduction in the early 20th century, primarily in ferromagnetism. Originally developed by Wilhelm Lenz and his student Ernst Ising in 1925, the model was used to explain phase transitions in magnetic materials. Over time, the model has been used in statistical mechanics, allowing researchers to explore phenomena such as phase transitions, in a variety of systems. In biology, the Ising model has been applied to understand protein folding, where amino acids interact similarly to spins in aligning or misaligning configurations.[5]

The Ising model is a powerful framework for mimicking phase separations in biological systems, particularly in lipid membranes. In lipid bilayers, molecules can exist in either an ordered or disordered state, similar to the two states of spins (up and down) in the Ising model. This allows the focus on the general properties of binary phase domains and how they influence each other. As temperature and environmental conditions change, lipid molecules experience phase transitions between these states. At higher temperatures, lipids are more fluid and disordered, resembling a paramagnetic state in the Ising model where spins are randomly oriented. As the temperature drops the lipids cluster. This clustering leads to phase separation, which plays a crucial role in processes like cell signaling and protein

sorting.[6] Understanding how physical models like the Ising model map onto biological processes can offer predictive tools for diagnosing or modeling diseases, such as neurodegenerative disorders linked to protein misfolding, thereby contributing to both theoretical and biomedical advancements.

2. Methods and Models

The code simulates a 2D Ising model using the Metropolis algorithm to study the behavior of magnetic spins on a lattice. The Ising model consists of spins that can take values of +1 or -1, and these spins interact with their nearest neighbors. The interaction energy between neighboring spins is determined by a coupling constant J, and an external magnetic field h is applied to the system. The temperature of the system is incorporated through the parameter kT, where $kT = kT_c \times (t + 1)$, with t controlling the deviation from the critical temperature T_0, the temperature at which the system undergoes a phase transition. The Metropolis algorithm is used to update the spins: at each step, a randomly selected spin is flipped with a probability determined by the energy difference between the current and proposed configurations. This allows the system to evolve toward equilibrium, accounting for thermal fluctuations. The program tracks the total spin S and the total lattice energy over a series of sweeps (simulation steps). The output includes plots of the spin sum and lattice energy over time.

Use of t and the Equation:

The parameter t is used in line 8 to calculate the temperature kT as:

$$kT = kT_c \times (t + 1)$$

Where $kT_c = \frac{1}{log(1+\sqrt{2})}$ is the critical temperature. This equation adjusts the system's temperature relative to Tc, and the resulting kT is used throughout the simulation to determine thermal effects on spin flips and energy updates. Specifically, kT influences the probability of flipping spins (via the inverse temperature) and the calculation of energy differences.

3. Results

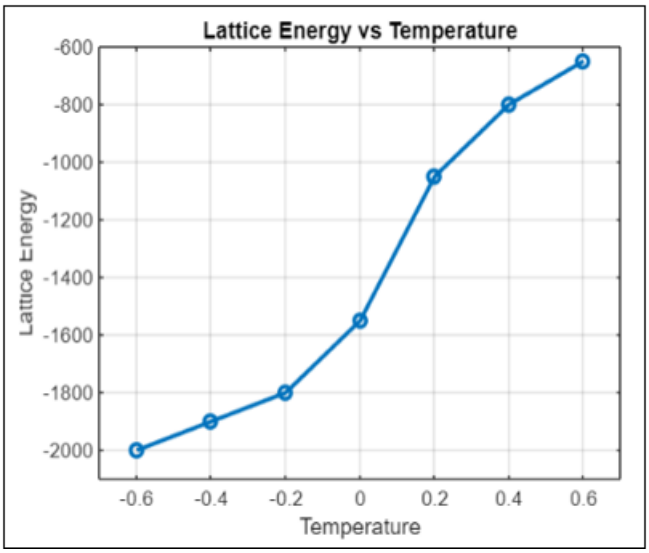

Figure 1: Graph depicting the relationship between lattice energy and temperature in the Ising Model. This visualization highlights phase transitions and critical points, offering insights into the thermodynamic behavior of spin systems

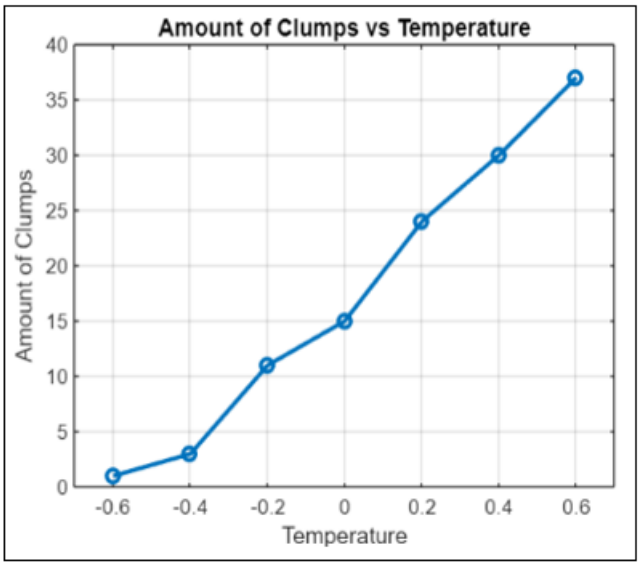

Figure 2: Graph depicting the relationship between the number of clumps and temperature in the Ising Model. This visualization highlights the effect of temperature on neighbouring spins

There is a clear relationship between temperature and the Ising model's spin count, as shown by the data in [Figure 2]. This relationship emphasizes how temperature can affect phase transitions, especially in systems with binary states, and is frequently seen in biological systems. The binary character of biological processes, such as the folding of biomolecules or the activation or deactivation of proteins, is illustrated by the spin-up and spin-down states of the Ising model. Understanding how temperature impacts the Ising model helps us better understand biological phenomena such as diseases caused by misfolded proteins or the control of cellular signaling networks. As the temperature decreases, proteins begin to fold more stably, forming ordered structures, similar to how the number of spins decreases as temperature decreases in the Ising model. This trend is observed in

neurodegenerative diseases like Alzheimer's or Huntington's, where lower temperatures cause proteins to misfold and aggregate into plaques or clumps.[3]

This study illustrates how the 2D Ising model, paired with the Metropolis algorithm, effectively simulates phase transitions in binary biological systems. The results not only mirror behaviors such as protein folding and lipid phase separation but also open the door to broader applications in disease modeling and cellular signaling. Future work could explore higher-dimensional models or integrate real biological data to enhance model accuracy.

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