# PHY480 Project 4: Ising Model

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**Abstract:** In this project we aim to explore phase transitions in two dimensions using the Ising Model with a Metropolis algorithm Monte Carlo method and periodic boundary conditions. We first used a 2x2 lattice to test the analytic solution, and then explored the results for larger lattices. We found that the system reached equilibrium faster at lower temperatures. The probability density at $T = 1$ is clustered tightly around the minimum energy and at $T = 2.4$ it is loosely arranged at a higher energy. To search for evidence of phase transitions, we used the Ising Model across a range of temperatures. We found that a critical temperature exists at $T_c \approx 2.25$. Lastly, we used our Ising Model code to do a runtime analysis using pure Python and Numba. At small lattice sizes, the pure Python code runs faster due to the overhead required by Numba, but Numba runs approximately twice as fast for larger lattices.

## I. INTRODUCTION

The Ising Model was developed by Ernst Ising to model ferromagnetism in two dimensions. In this model, dipole moments (which can either be -1 or 1) are arranged in an $nxn$ lattice and are allowed to interact with their neighbors.

A Monte Carlo algorithm, in this case the Metropolis algorithm, is then used to simulate the changing magnetism of the system. In each iteration of our implementation, we randomly select a dipole in the lattice and calculate the energy of its nearest neighbors. Based on this energy and the probabilities of changing energies, the dipole is either switched or remains the same. Through many iterations, the system tends towards equilibrium, which is a ferromagnetic system.

The Ising Model allows for the study of phase transitions, and due to its simplicity is a widely used model in statistical mechanics. We implement the Ising Model with periodic boundary conditions for a 2x2 lattice to confirm the analytic results and then tested the accuracy and runtime for 20x20 and 80x80 lattices.

## II. THEORY

The degeneracy, energy, and magnetization for a 2x2 lattice with periodic boundary conditions is listed in Table I. With these values, we will be able to calculate energy expectation value, mean magnetization, specific heat, and susceptibility as functions of temperature.

The partition function of an ensemble of spins can be written as

$$Z = \sum_i e^{-\beta E_i} \tag{1}$$

where $\beta = \frac{1}{K_B T}$, $K_B$ is the Boltzman constant, T is temperature, and $E_i$ is the energy of a microstate. Using the values above for our 2x2 lattice, the partition function is found to be

$$Z = 2e^{-8J\beta} + 2e^{8J\beta} + 12 = 4cosh(8\beta J) + 12 \tag{2}$$

Using the partition function, we can find the expectation value of energy using

$$\langle E \rangle = -\frac{\partial ln(Z)}{\partial \beta} \tag{3}$$

$$-\frac{J(16e^{8J\beta} - 16e^{-8J\beta})}{2e^{-8J\beta} + 2e^{8J\beta} + 12} = -\frac{8Jsinh(8J\beta)}{cosh(8J\beta) + 3}$$

Next, we can find the mean magnetization with

$$\langle M \rangle = \sum_i \frac{M_i e^{-\beta E_i}}{Z} \tag{4}$$

Using the equations from Table I, we found that $\langle M \rangle = 0$ The specific heat is given by

$$C_v = \frac{\langle E^2 \rangle - \langle E \rangle^2}{K_B T^2} \tag{5}$$

First we find $\langle E^2 \rangle$ using

$$\langle E^2 \rangle = \sum \frac{e^{-\beta E_i} E_i^2}{Z} = \frac{64J^2 cosh(8J\beta)}{cosh(8\beta J) + 3} \tag{6}$$

With this we are able to find the specific heat to be

$$C_v = \frac{64J^2}{K_B T^2 (cosh(8J\beta) + 3)} \left( cosh(8J\beta) - \frac{sinh^2(8J\beta)}{cosh(8J\beta) + 3} \right) \tag{7}$$

| Spins Up | Degeneracy | Energy | Magnetization |
|---|---|---|---|
| 4 | 1 | -8J | 4 |
| 3 | 4 | 0 | 2 |
| 2 | 4 | 0 | 0 |
| 2 | 2 | 8J | 0 |
| 1 | 4 | 0 | -2 |
| 0 | 1 | -8J | -4 |

TABLE I. A table showing the degeneracy, energy, and magnetization for all microstates in a 2x2 lattice of spins with periodic boundary conditions

The susceptibility is given by by the following equation

$$\chi = \frac{\langle M^2 \rangle - \langle M \rangle^2}{K_B T} \tag{8}$$

First we will calculate $\langle M^2 \rangle$ with

$$\langle M^2 \rangle = \frac{e^{-\beta E_i} M_i^2}{Z} = \frac{8e^{8J\beta} + 8}{cosh(8J\beta) + 3} \tag{9}$$

From here we find

$$\chi = \frac{1}{K_B T} \frac{8e^{8J\beta} + 8}{cosh(8J\beta) + 3} \tag{10}$$

## III. RESULTS

### A. The 2x2 Lattice

We wrote an Ising model code to simulate a 2x2 lattice of spins. We aimed to check our simulation code with our theoretical calculations, so we calculated $\langle E \rangle$,$\langle E^2 \rangle$,$\langle M \rangle$, and $\langle M^2 \rangle$ from our code. We were able to do this by running 500 simulations with random initial conditions and calculating the mean and variance of energy and magnetization for various temperatures.

To get an estimate for the number of Monte Carlo cycles we needed to run, we let T = 1 in our code and compared the results to T = 1 for the theoretical equations. We found that 25 cycles was enough to get good convergence. Figures 1-4 show the comparison of our theoretical predictions to our simulated results.

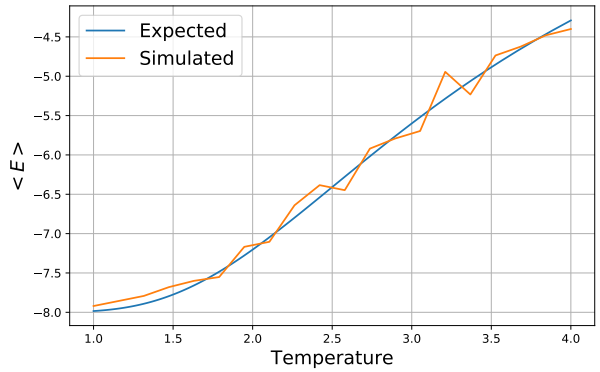


FIG. 1. A comparison of our calculated and simulated energy expectation value as a function of temperature

As you can see for $\langle E \rangle$,$\langle M \rangle$, and $\langle M^2 \rangle$, our simulation fully agrees with the theoretical results. Due to the stochastic elements of our simulation there is a little noise, but all around follows the same trends.

However our simulation is very far from the theoretical prediction for $\langle E^2 \rangle$. We believe this is due to the fact the simulation is only a 2x2 lattice. So at low temperatures

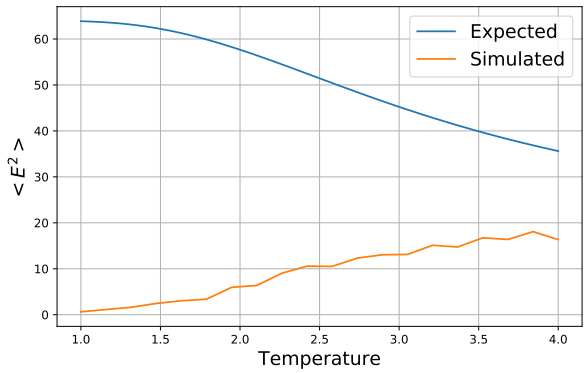


FIG. 2. A comparison of our calculated and simulated energy variance as a function of temperature

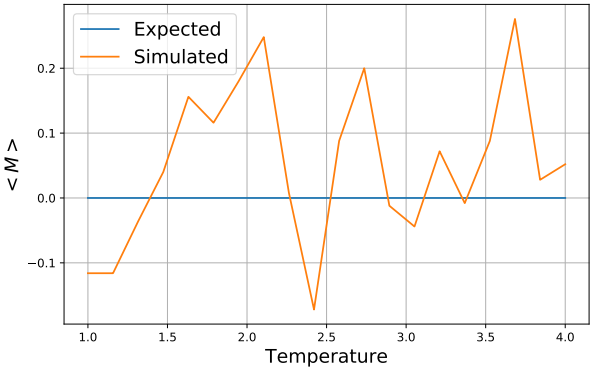


FIG. 3. A comparison of our calculated and simulated magnetization expectation value as a function of temperature

25 Monte Carlo cycles is more than enough for the system to come to equilibrium.

Comparing our calculated and predicted $C_v$ and $\chi$ unsurprisingly we found that there was good agreement in $\chi$ since the measurements for $\langle M \rangle$ and $\langle M^2 \rangle$ where close to the expected. Since our simulated $\langle E^2 \rangle$ was so far from the expected, it is unsurprising that the specific heat we calculated was far off from expected. These comparisons can be seen in Figure 5 and 6

### B. Equilibrium Convergence Rate

To explore the needed number of Monte Carlo cycles we looked at the expectation value for energy and magnetization as a function of cycles. We looked at the T = 0 and T = 2.4 case for a randomly initialized lattice, and an order lattice where all the spins start pointing down. To calculate the expectation values for the simulation, we ran it with the chosen initial condition for 100 trials. The mean of the energy and magnetization distributions are

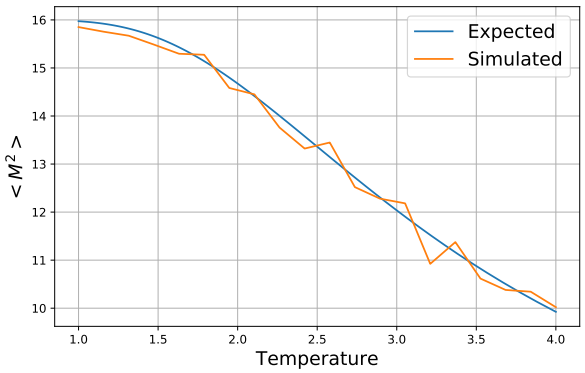


FIG. 4. A comparison of our calculated and simulated magnetization variance value as a function of temperature

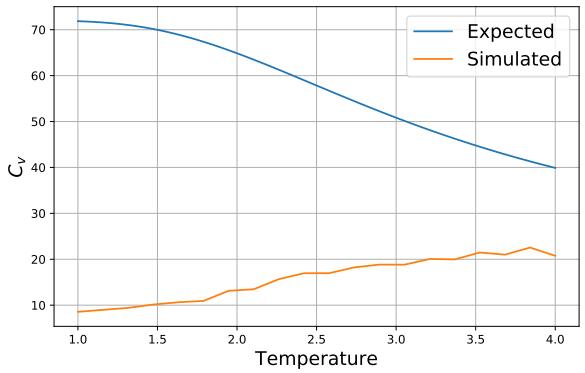


FIG. 6. A comparison of our calculated and simulated specific heat as a function of temperature

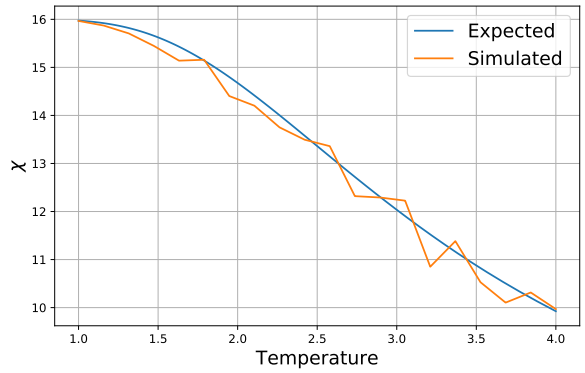


FIG. 5. A comparison of our calculated and simulated susceptibility as a function of temperature

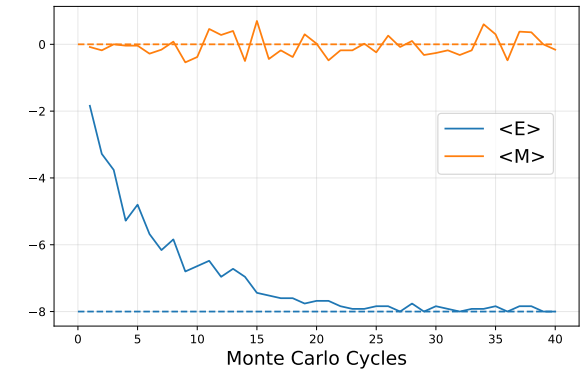


FIG. 7. The expectation values for energy and magnetization as a function of Monte Carlo cycles for a randomly initialized system at T = 1

the expectation values for the respective quantity.

### C. T = 1, Random Initial Condition

When the system is randomly initialized and has a temperature of 1, it takes about 25 Monte Carlo cycles for the energy expectation value to settle to the predicted value. The magnetization expectation value is close to the predicted value for all number of Monte Carlo cycles. These results can be seen in Figure 7 .

### D. T = 1, All Up Initial Condition

If we initialize the system with all of the spins pointing up with a temperature of 1, we find that the energy for any number of cycles is producing the expected result. Even after 500 cycles, the magnetization is nowhere near zero, this is not surprising though, since we are initializing the system to have a net magnetization of 4 each run. These results can be seen in Figure 8.

### E. T = 2.4, Random Initial Condition

In the case where we initialized the system randomly at a temperature of 2.4, we once again saw that the magnetization was where we expected for any number of cycles. It took about 20 cycles until the energy expectation value settled to the expected value. These results can be seen in Figure 9.

### F. T = 2.4, All Up Initial Condition

When we initialized the system to have all spin up at a temperature of 2.4, we saw that the energy settles in approximately 20 cycles and the magnetization took about 120 cycles. These results can be seen in Figure 10. For a system that is randomly initialized, we can see

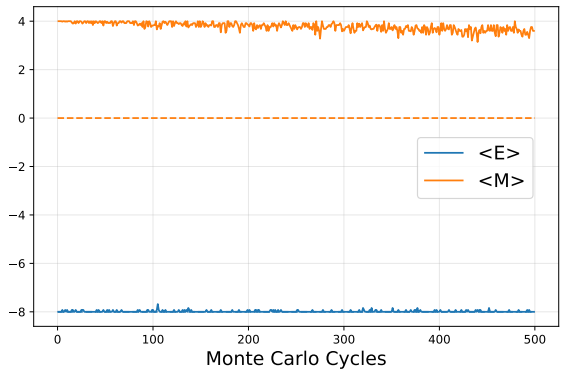


FIG. 8. The expectation values for energy and magnetization as a function of Monte Carlo cycles for a system initialized with all spins pointing up at T = 1

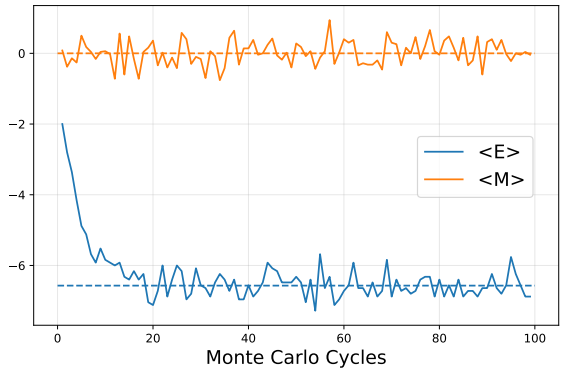


FIG. 9. The expectation values for energy and magnetization as a function of Monte Carlo cycles for a randomly initialized system at T = 2.4

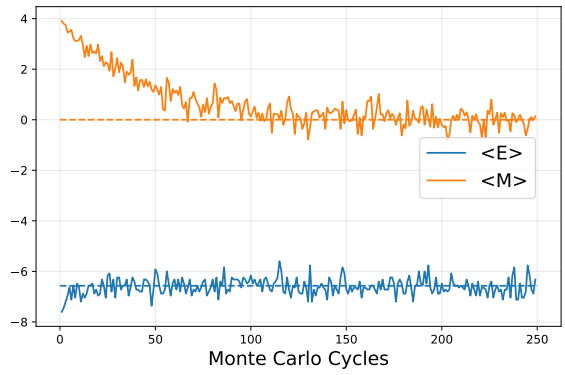


FIG. 10. The expectation values for energy and magnetization as a function of Monte Carlo cycles for a system initialized with all spins pointing up at T = 2.4

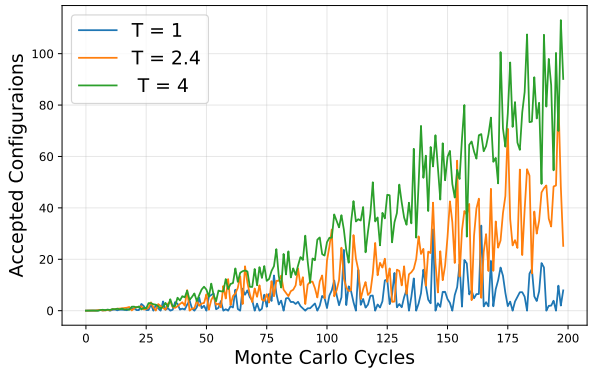


FIG. 11. A comparison of the number of accepted configurations as a function of Monte Carlo cycles. The results for 3 different temperatures can be seen.

how the number of accepted configurations depends on temperature and the number of cycles in Figure 11. As you can see, as temperatures rise more configurations are accepted. The system is more likely to go to a state with a higher energy when it has a higher temperature, so it is more likely to accept configurations. The green T = 4 curve for example is accepting around half of the configurations it tries, while the blue T = 1 consistently only accepts 10 - 20 configurations regardless of the number of cycles it goes through.

### G. Probability Density

In this section we aimed to sample the probability distribution of states. We wanted to sample the distribution at a temperature of 1 and 2.4. We started by setting up a 20x20 lattice of spins, and ran our code for 20000 cycles. We counted the energies we found after equilibrium was established. We found the distribution in Figure 12 and also plotted it on a logarithmic scale in Figure 13.

The probability at T = 1 has a varience of 10.3, while at T = 2.4 it is 3453. It is quite apparent at low temperatures that most simulations end up with all spins aligned and a minimum energy at -800. There is a small fluctuation where a hump forms near -700. When the system is heated to T = 2.4, the distributions of energies spreads way out, and tends to a higher energy. This shows that at this temperature that the spins are mixing, and the system is unable to come to a state where the spins align to minimize the energy.

### H. Phase Transitions

In this section we are looking for evidence of phase transitions with our code. By running our code over a temperature range and calculating various expectation values, we can look for changes in behavior consistent with a phase transition.

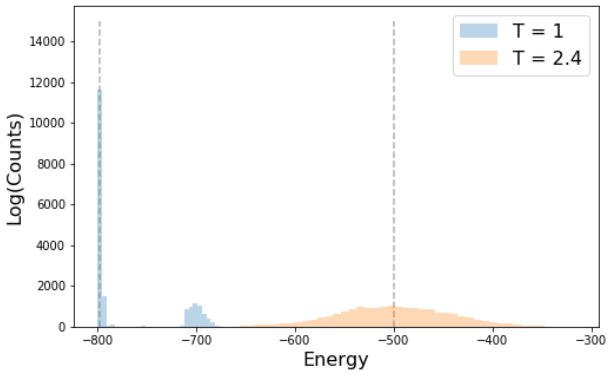


FIG. 12. Probability distributions of the Ising model at a temperature of 1 (blue) and 2.4 (orange). The mean of the distributions is shown by black dotted lines.

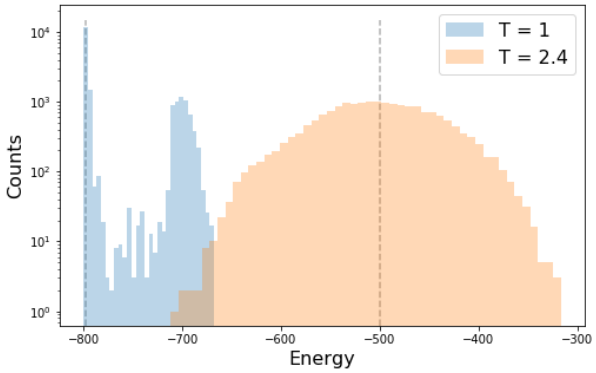


FIG. 13. Probability distributions of the Ising model on a logrithmic scale at a temperature of 1 (blue) and 2.4 (orange). The mean of the distributions is shown by black dotted lines.

We varied the temperature between 1 and 4 degrees and plotted the energy expectation value in Figure 14. We averaged many runs to get a smoother curve. Due to the stochasim in the code a single run is very noisy. Around 2.4 degrees, the curve for the energy expectation value switches concavity and starts to approach an asymptote.

We varied the temperature in a similar way while measuring the net mean magnetization. At low temperatures, it held a pretty constant value with most of all the spins pointing in the same direction. As the temperature raised, the net magnetization began to fall around 2.4 degrees. By 3 degrees, the net magnetization was approximately zero meaning there was a even mix of up and down spins and no domains were forming. These results can be seen in Figure 15 This sudden change in magnetization shows a change in the behavior of the system. Below this critical temperature the system tends to form domains and fall into an equilibrium with all of the spins aligned. Past the critical temperature, the the system is unable to align itself, and the spins are pointing in random direction,

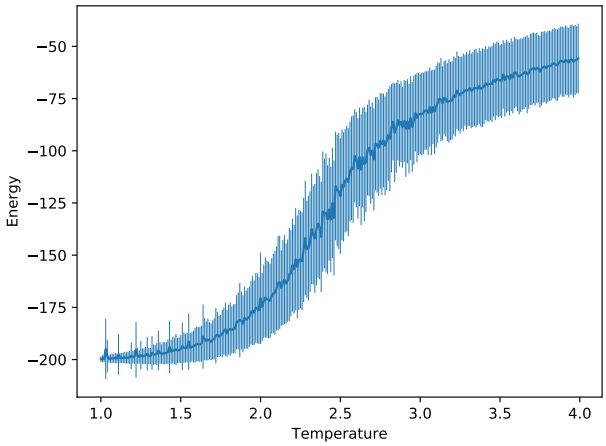


FIG. 14. The energy expectation value of our ising model as a function of temperature. The energy changes concavity around 2.4 degrees showing evidence of a phase transition.

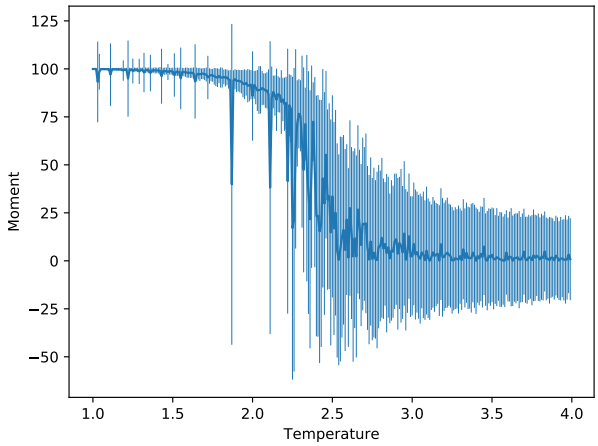


FIG. 15. The absolute magnetization of our simulation as a function of temperature. Around 2.4 degrees the net magnetization suddenly tends to zero.

leading to the overall lack of magnetization. This critical temperature is known as the Curie temperature where a material losses its magnetic properties due to the mixing of spins.

## I. Critical Temperature

In the previous section, we saw that there was a critical temperature where the behavior of our system changed. Using our runs and the resulting plots of the energy and magnetization expectation values, we estimated the critical temperature for our ising model as the side length heads to infinity. We took steps in temperature at a size

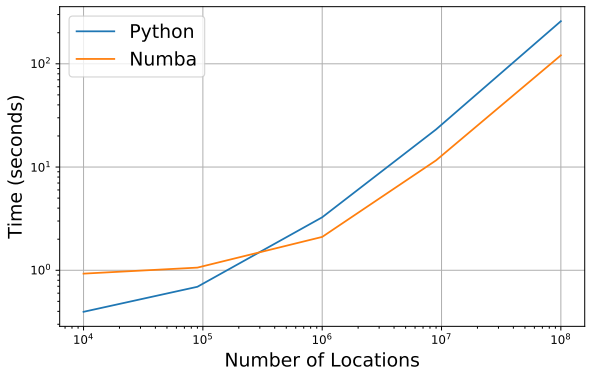


FIG. 16. A timing study of pure Python vs Numba for our ising model code.

of .01. Through our simulation, we determined that the critical value was approximately 2.25. Lars Onsager was able to find the exact result for the critical temperature to be $2/\ln(1+\sqrt{2}) \approx 2.269$[1]. With finer time steps we would be able to get a better approximation.

### J. Large Scale Simulation

We did a relatively large scale simulation of a 500x500 lattice. We let it run for 2.5x$10^7$ steps and the magnetism at select steps can be found in Figures 17-21 at the end of this document. From these figures the domains forming can clearly be seen as local variation is decreasing.

## IV. RUNTIME ANALYSIS

We wanted to explore the speed of our code, and compare the results of using pure Python vs Numba-ed Python. The results of this study can be seen in Figure 16. To preform this study, we ran our code with and without Numba for 500 time steps, and varied the side length of our square lattice. As you can see at small lattice sizes, the overhead of using Numba actually makes our code slower compared to using pure Python. This result is generally expected in the small size limit. Past the 2x$10^5$ locations point, Numba runs about twice as fast as pure Python.

## V. CONCLUSION

We wrote code for an Ising Model simulation of ferromagnetism in two dimensions using the Metropolis algorithm as the underlying Monte Carlo method and tested it for various lattice sizes. To ensure the code was working properly, we analytically solved the Ising model for a 2x2 system and showed that our results matched our theory.

We then used a 20x20 lattice to sample a probability distribution and study phase transitions. At low temperatures, the probability distribution is clustered tightly at the minimum energy of the system. As the temperature increases, the probability distribution spreads out significantly and is centered at a higher energy showing the spins are not aligning and forming domains.

Using our Ising model code, we found evidence of a phase transition (energy leveling off and the magnetic moment tending towards zero). We found the the phase transition occurred at a critical temperature $T_c \approx 2.25$, which was very close to the expected result of 2.269 [1].

Finally, we compared the runtime of our model using pure Python and Python with Numba. We found that Numba is slower at small lattice sizes due to significant overhead as expected, but it is approximately twice as fast as pure Python at large lattice sizes.

[1] L. Onsager. Crystal statistics. i. a. a two-dimensional model with an order-disorder transition. *Physical Review*, 1943.

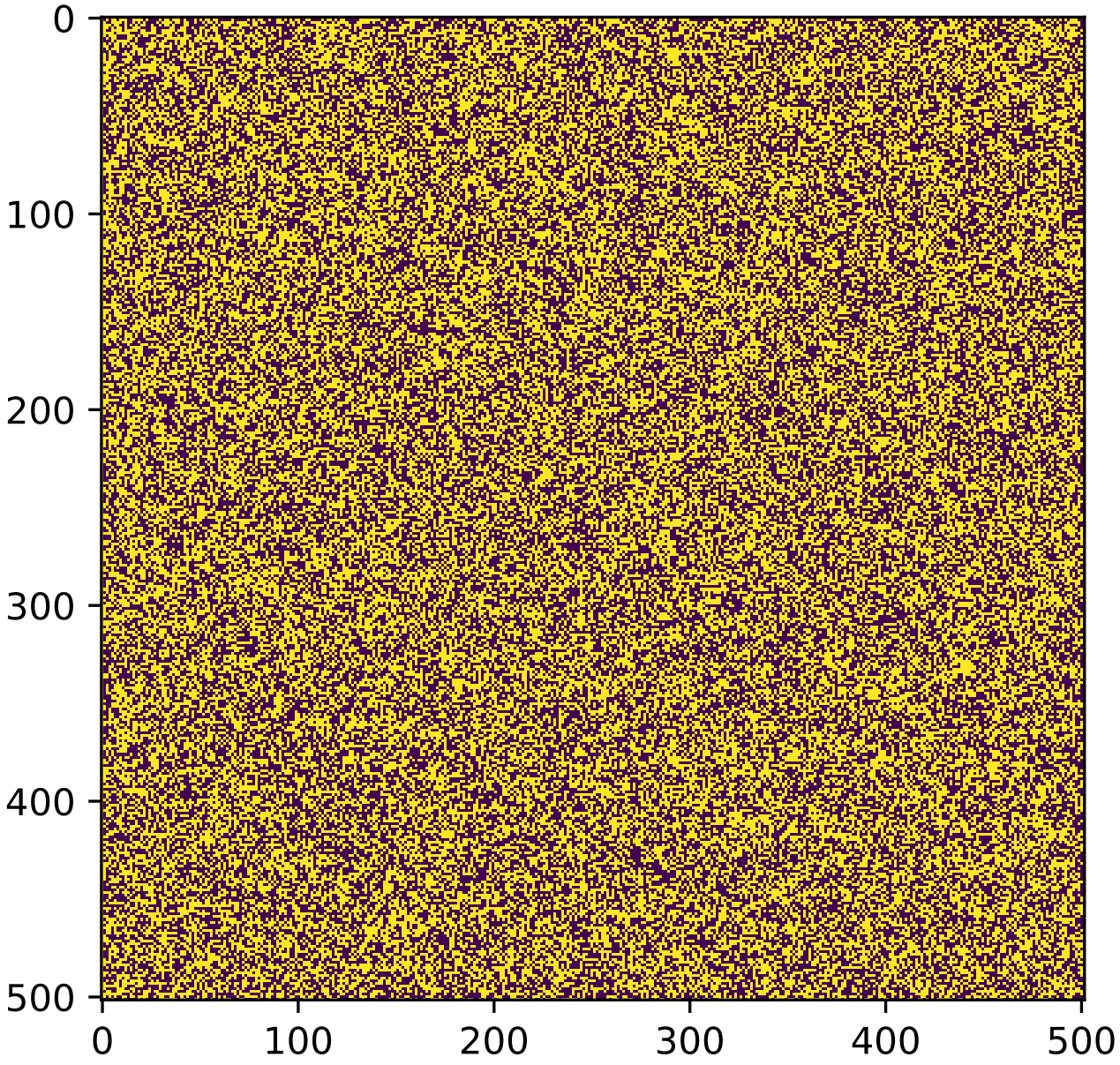


FIG. 17. Step=0

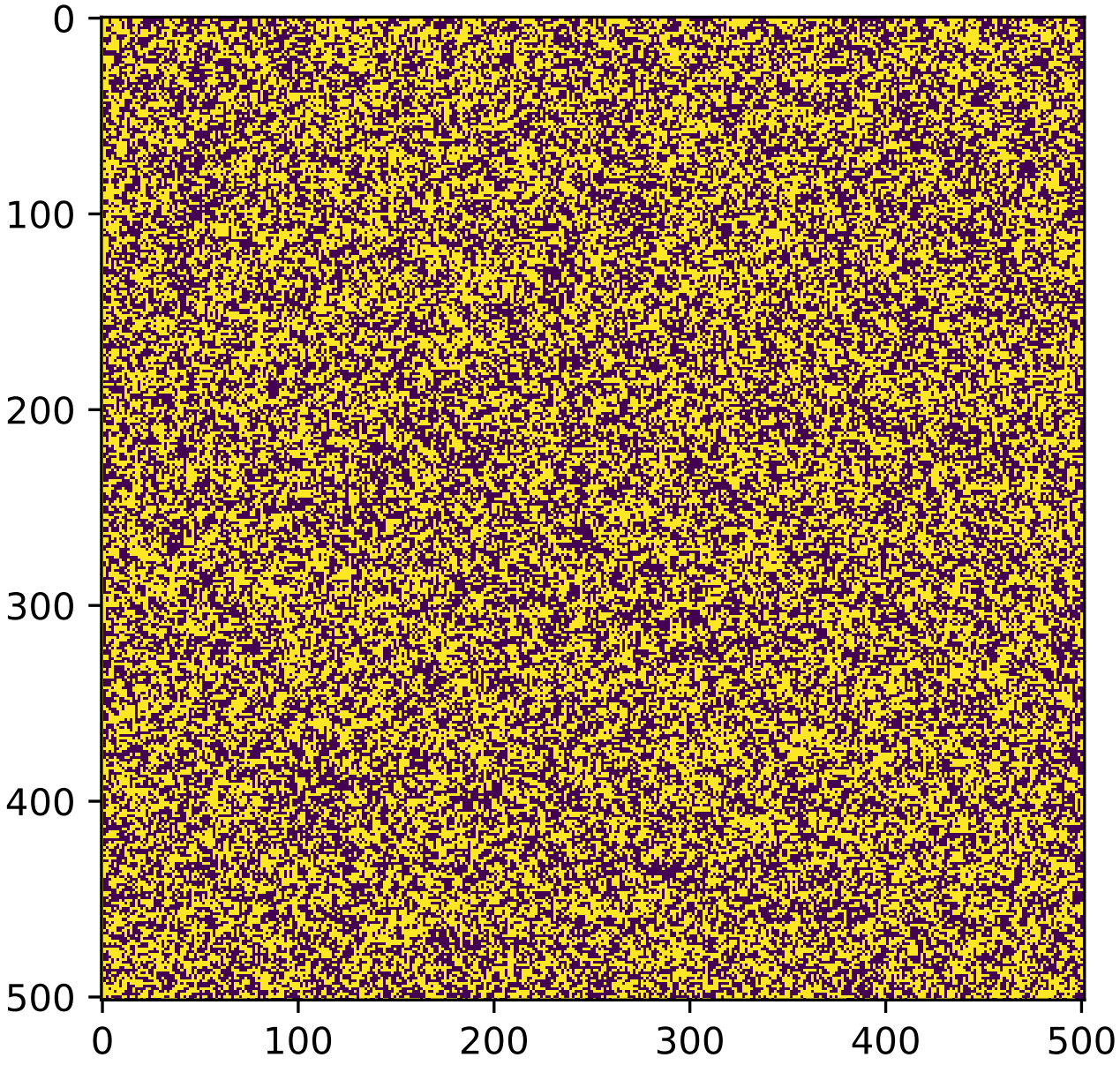


FIG. 18. Step=$10^5$

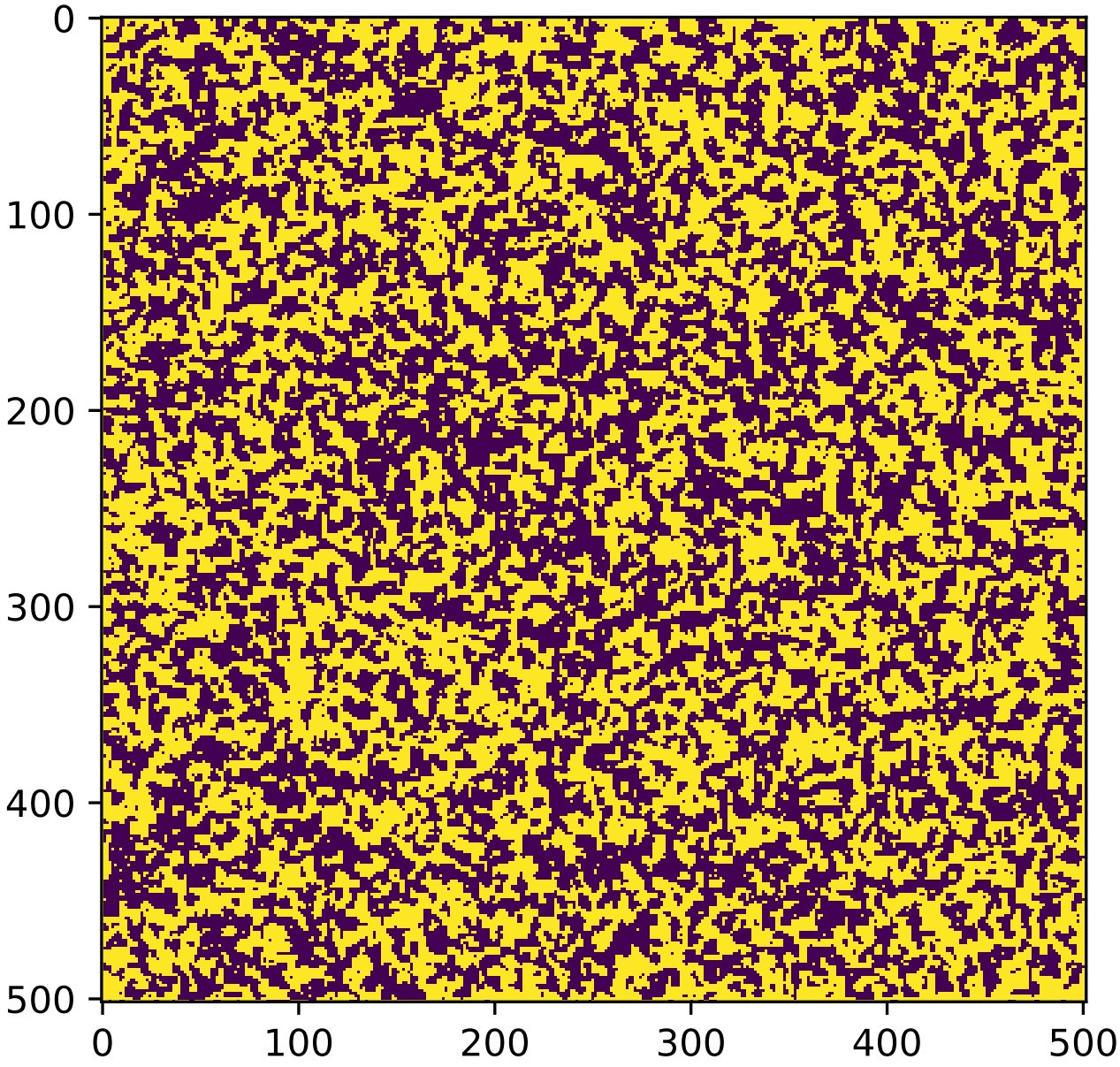


FIG. 19. Step=$10^6$

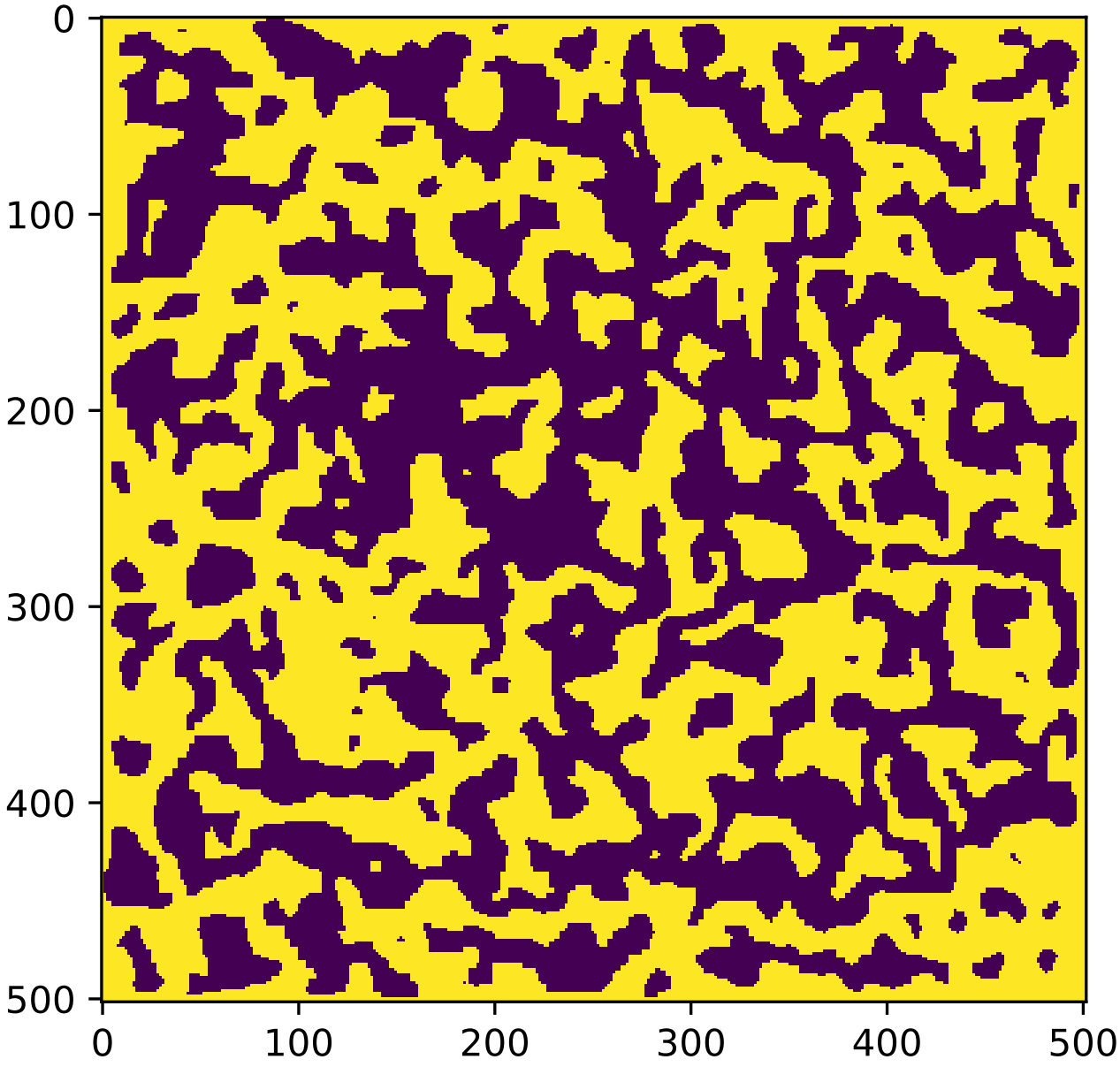


FIG. 20. Step=$10^7$

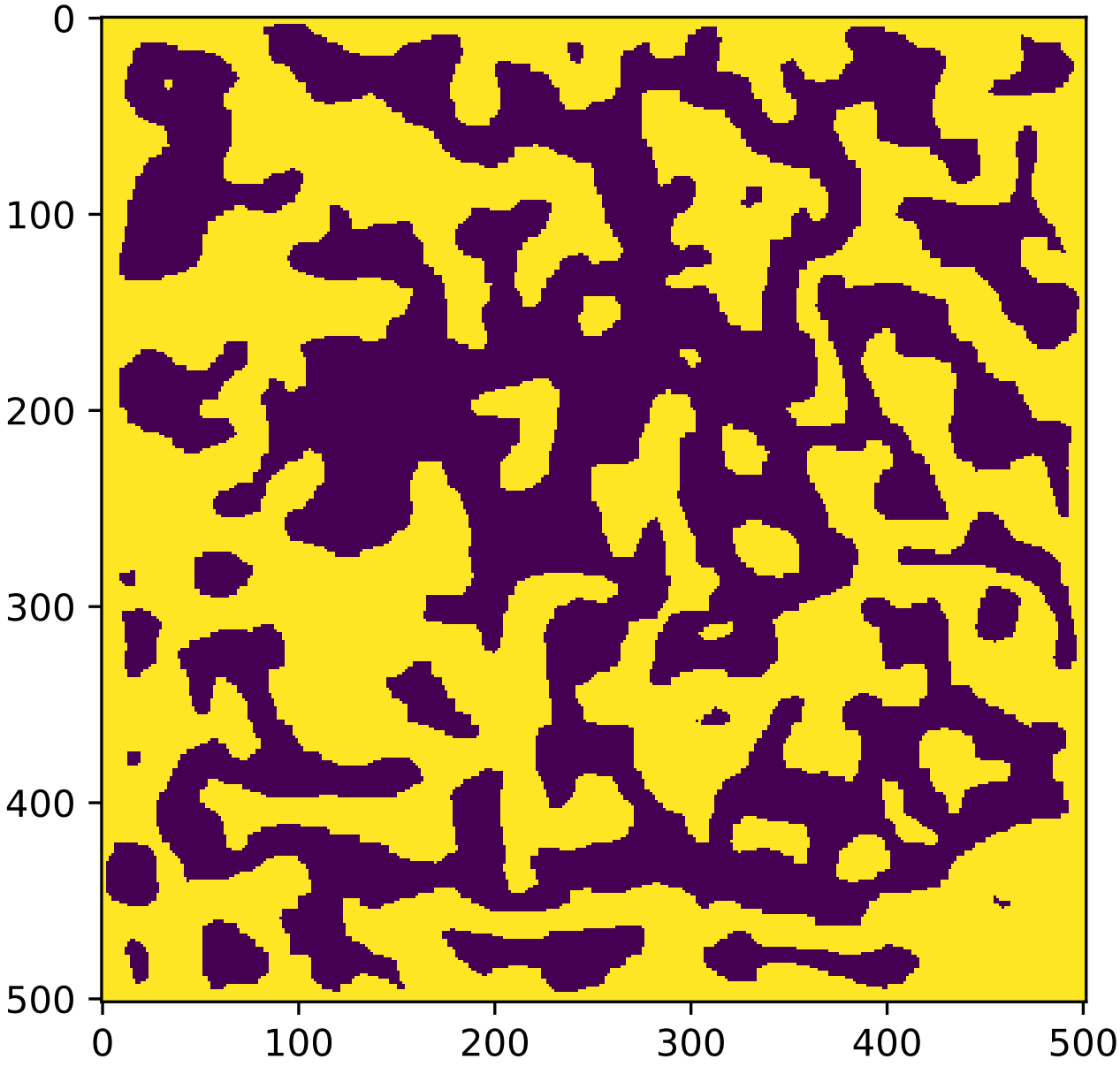


FIG. 21. Step=$2.5 \cdot 10^7$