Metropolis Monte Carlo simulation of the Ising Model

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Modelling and Simulation of Particulate Processes (CH5012)

Introduction

- The Ising model, developed by Dr. Ernst Ising is used for modelling ferromagnetic and anti-ferromagnetic materials
- The model represents a lattice occupied by atoms which can each have dipole moments or spins
- The model predicts a second order phase transition occuring at the Curie temperature for dimensions higher than 1
- Phase transition is identified from ensemble properties and compared with the theoretical model which has been solved exactly for zero external field

Ferromagnetism

- One of the fundamental properties of an electron is that it has a dipole moment
- This dipole moment comes from the more fundamental property of the electron that it has quantum mechanical spin
- The quantum mechanical nature of this spin causes the electron to only be able to be in two states, with the magnetic field either pointing "up" or "down"
- When these tiny magnetic dipoles are aligned in the same direction, their individual magnetic fields add together to create a measurable macroscopic field

Ferromagnetism

- Ferromagnetic materials are strongly ordered and have net magnetization per site as $-1/1$ under temperatures $T < T_c$
- They are able to maintain spontaneous magnetization even under the absence of external fields
- At temperatures above T_c, the tendency to stay ordered is disrupted due to competing effects from thermal motion
- The ferromagnetic substance behaves like a paramagnetic substance at $T > T_C$, showing no spontaneous magnetization

Ferromagnetism

- The reason for this strong alignment/bonding arises from exchange interactions between electrons
- These exchange interactions are $\approx$1000 times more stronger than dipole interactions, characteristic of paramagnetic and diamagnetic substances
- In antiferromagnetic materials, these exchange interactions tend to favor the alignment of neighbouring atoms with opposite spins
- As far as the Ising Model goes, coupling parameter $J > 0$ for ferromagnetic substances and $J < 0$ for antiferromagnetic substances

Hamiltonian

- Each atom can adopt two states, corresponding to $s = \{-1, 1\}$, where s represents the spin and the spin interactions are dependent on the coupling parameter J_{ij}
- The lattice model has periodic boundary conditions and extends infinitely
- This model is defined in the Canonical Ensemble(N, V, T) and the *Hamiltonian* is defined as below

$$H = -J_{ij} \sum_{<i\,j>} s_i s_j - h \sum_i s_i$$

where,
J_{ij}= Coupling parameter between the adjacent atoms
h = External Field Strength
$s_{i,j}$ = Spin of particle

Partition Function

The Partition function corresponding to the Hamiltonian for the above model is defined as:

$$Q_{partition} = \sum_{states} e^{-\beta H}$$

where $\beta = \frac{1}{k_b T}$, $k_b \rightarrow$ *Boltzmann Constant*

Ising 2-D Square Model

For an isotropic case, where the coupling along the rows and columns are equal, the critical temperature has been found to be

$$\frac{k_B T_c}{J} = \frac{2}{ln(1+\sqrt{2})} \approx 2.269$$

The 2-D square model in the absence of an external field has been solved (Lars Onsager, 1944) in the absence of an external field ($h = 0$)
Internal Energy:

$$U =< H >= \frac{\sum_{states} He^{-\beta H}}{Q_{partition}}$$

Isothermal Susceptibility:

$$\chi_T = (\frac{dM}{dh})_h = \frac{1}{k_B T}(< M_v^2 > - < M_v >^2)$$

Ising 2-D Square Model

Specific heat at constant volume:

$$C_v = (\frac{dU}{dT})_h = \frac{(< H^2 > - < H >^2)}{k_B T^2}$$

Net magnetization per particle:

$$k = \frac{1}{sinh(\frac{2J}{k_B T})sinh(\frac{2J^*}{k_B T})}$$

Spontaneous Magnetization per site, for $T < T_c$(isotropic):

$$M = [1 - sinh^{-4}(\frac{2J}{k_B T})]^{\frac{1}{8}}$$

Energy per site :

$$U = -Jcoth(\frac{2J}{k_B T})[1+\frac{2}{\pi}(2tanh^2(\frac{2J}{k_B T})-1)\int_0^{\frac{\pi}{2}} \frac{1}{\sqrt{1-\frac{4k}{(1+k)^2}sin^2(\theta)}}d\theta$$

Applicability of Monte Carlo simulations

- The rationale behind Monte Carlo sampling techniques is inherently based on the sampling of time steps from an exponentially distributed function and making stochastic decisions
- Since the Canonical ensemble arises from an exponential distribution of states, a similar rationale can be used to sample across the different states of the system until equilibrium is reached

Setting up the Problem

- An optimal value of 900 atoms was chosen to model this system with periodic boundary conditions
- The lattice was represented by a 31×31 random matrix, with each element being randomly assigned with the values -1 or 1

It is chosen as a 31×31 matrix so as to ensure that all the edges are periodic in nature. The values at the first and last column, first and last row are made the same

Setting up the Problem

- All quantities are manipulated in normalized units
- Temperature is normalised and $k_B \sim 1$ unit. The coupling strength is taken as $J = 1$ unit
- The whole procedure was done for different temperatures ranging from $0.5 - 3$ and the number of iterations for equilibration was taken as $n \approx 10^8$

Initial Lattice Structure

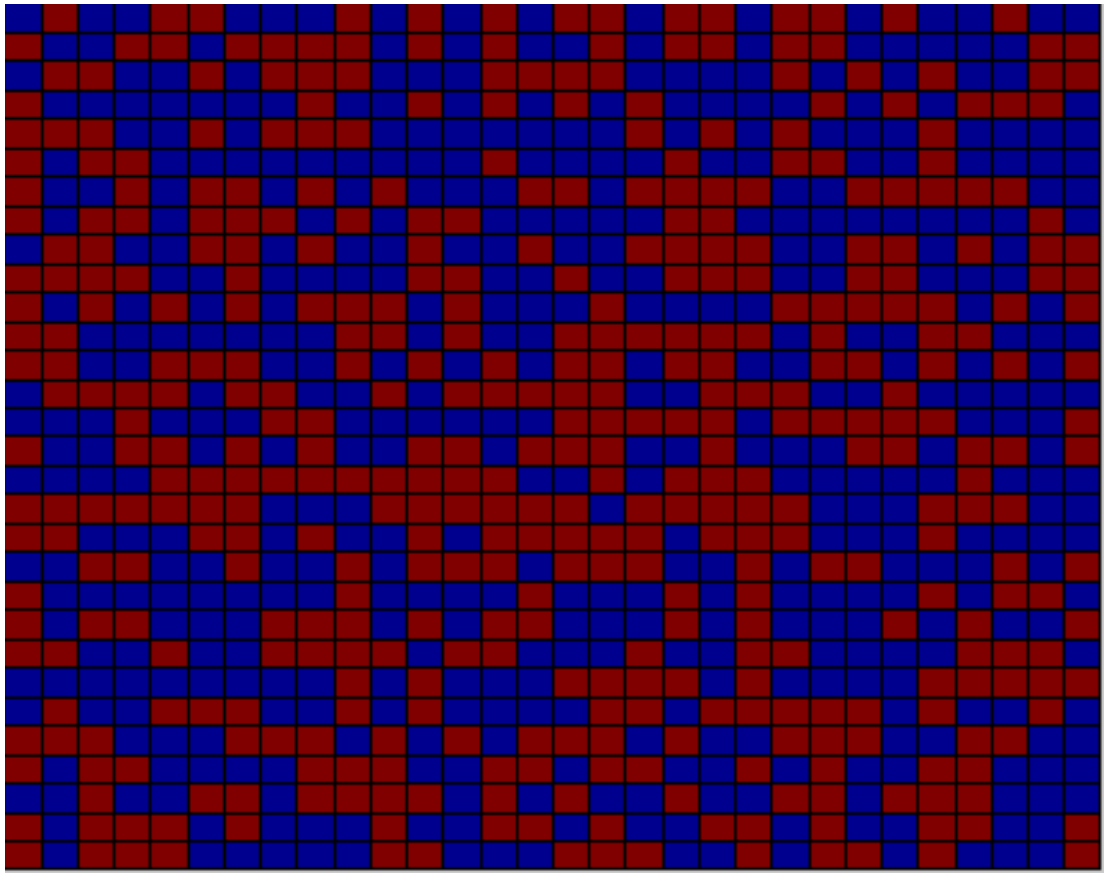

Figure: Intial lattice, blue squares represent $s = 1$ and red squares represent $s = -1$

Algorithm

- Initialise the system randomly with spins, at a given Temperature
- Set the value of the external field, in most cases $h = 0$
- Make a random flip in the spin of some atom
- Compute the Energy change arising from this, due to only the neighbouring atoms
- Ensure that the periodic boundary conditions are in place to take care of edge effects
- If $\triangle E < 0$, accept this configuration and continue this process

Algorithm

- If $\triangle E > 0$, accept this configuration with a probability of $p = exp(-\frac{\triangle E}{k_B T})$, else retain the old configuration
- Once every m, iterations , sample the system for important ensemble properties
- This sampling has to be done after discarding the edges because they only represent the periodic boundary conditions
- Now allow the system to equilibriate (typically takes $\sim n^3$ *iterations*)
- Estimate the average properties, variance terms(Susceptibility and C_v)
- Repeat this procedure at different temperatures

Visualization of MMC

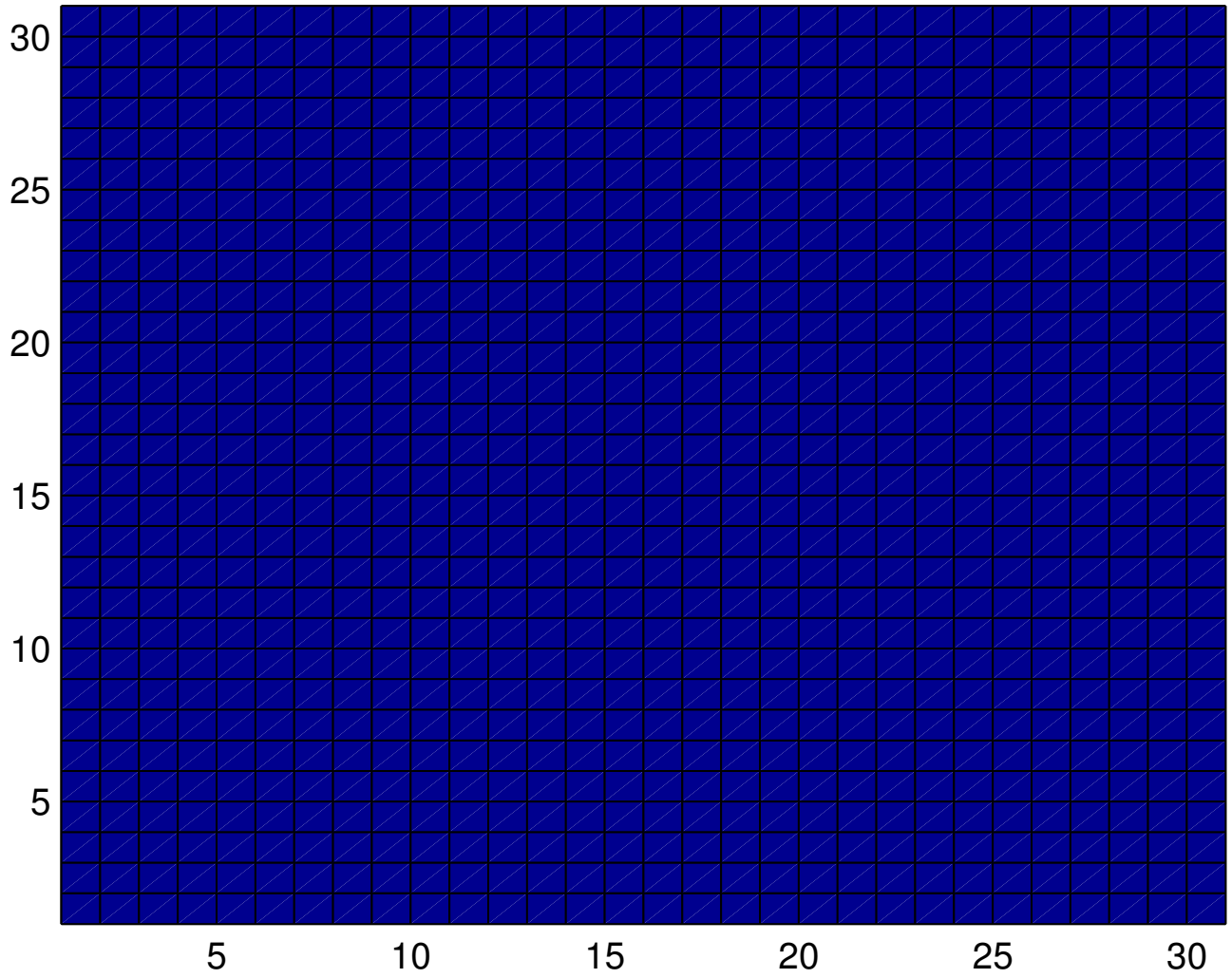

Figure: $T = 0.5$

Visualization of MMC

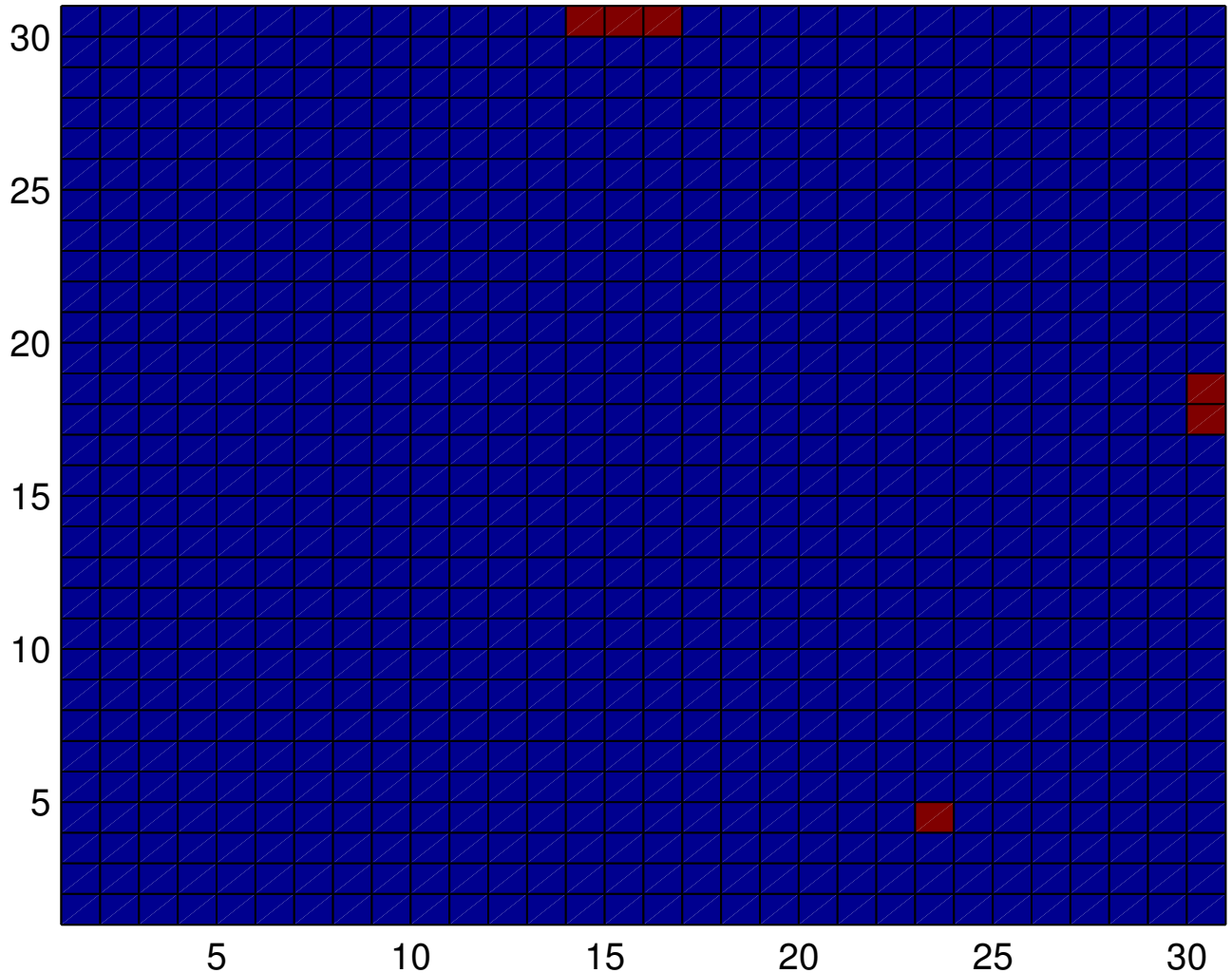

Figure: $T = 1$

Visualization of MMC

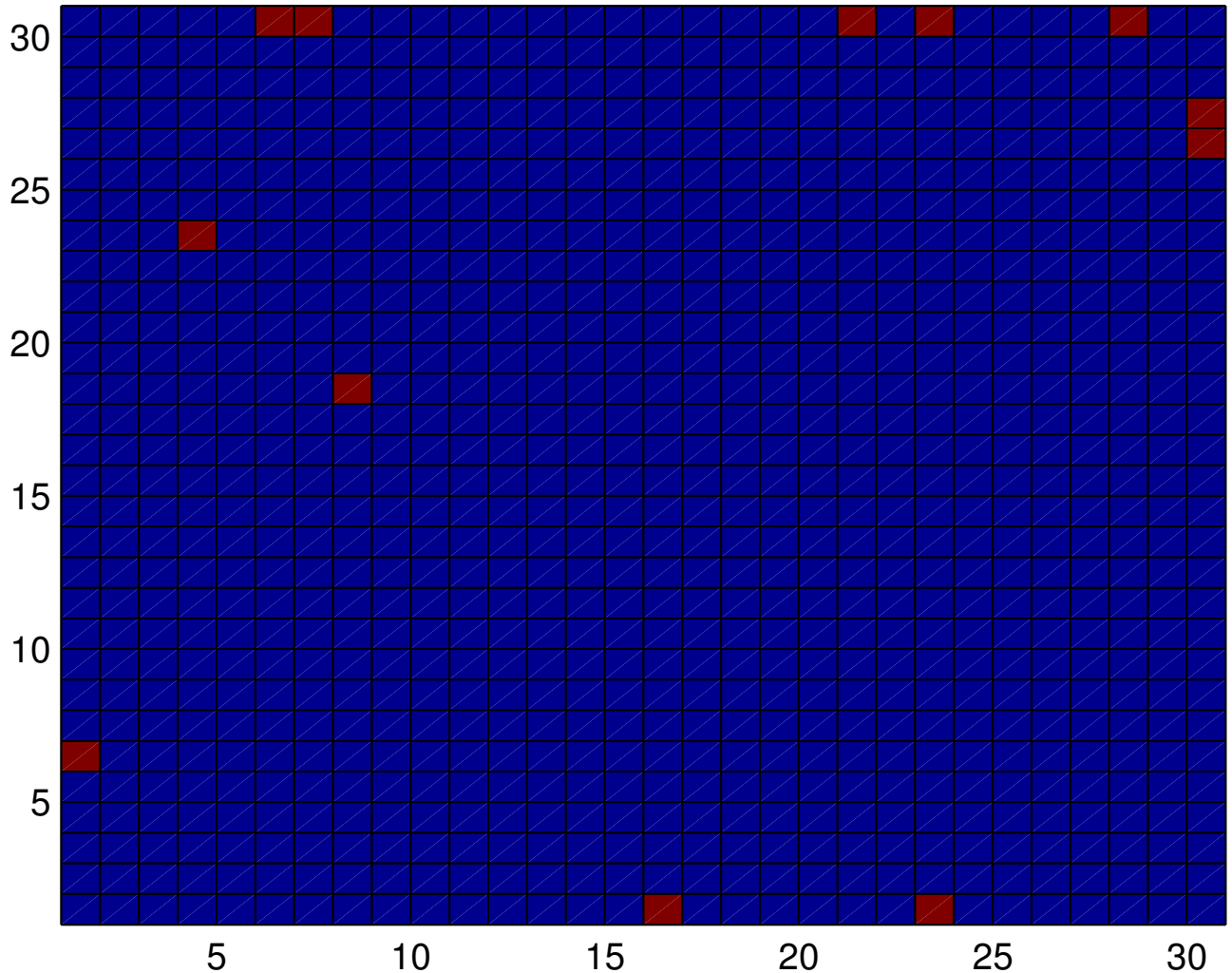

Figure: $T = 1.5$

Visualization of MMC

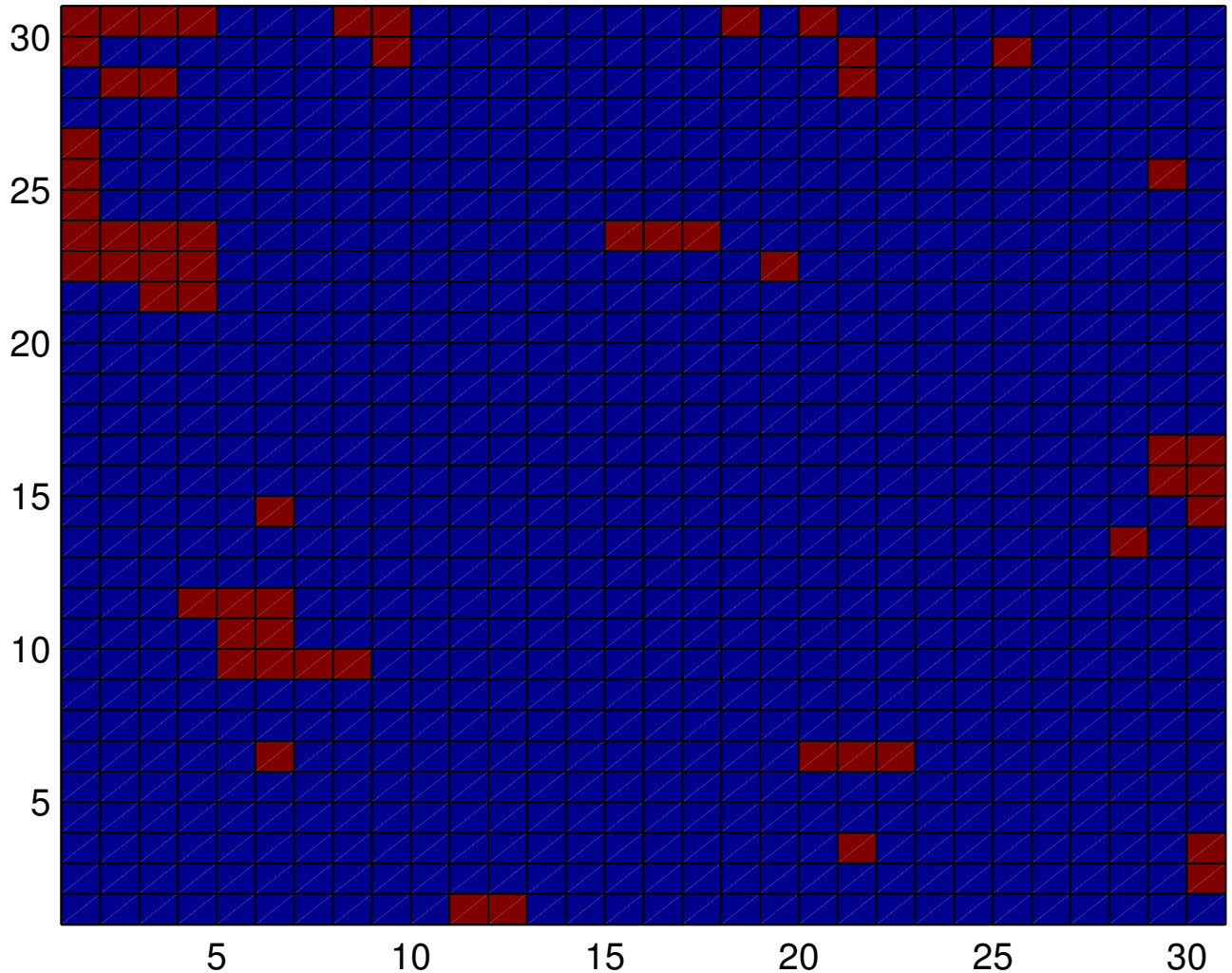

Figure: $T = 2$

Visualization of MMC

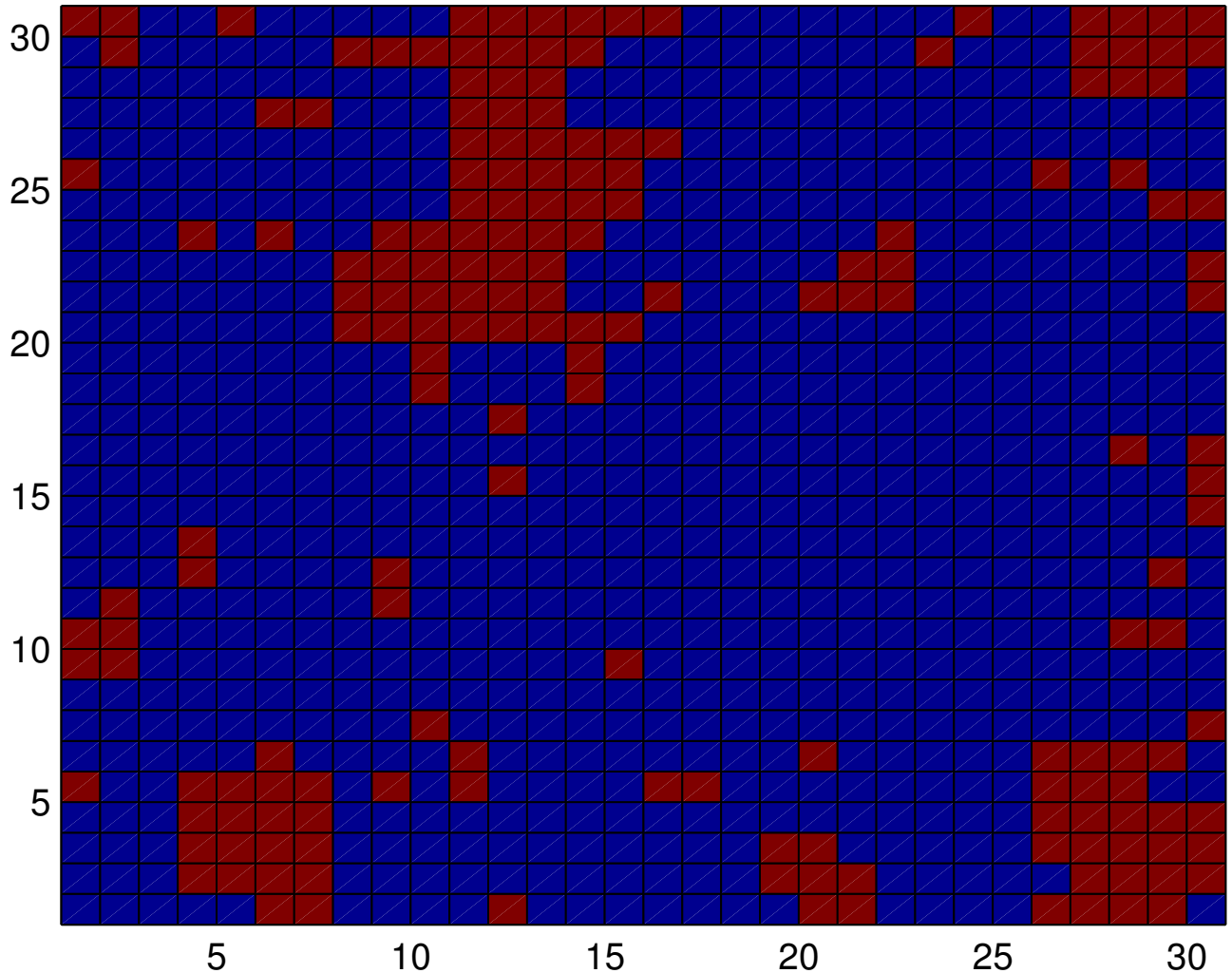

Figure: $T = T_c \approx 2.269$

Visualization of MMC

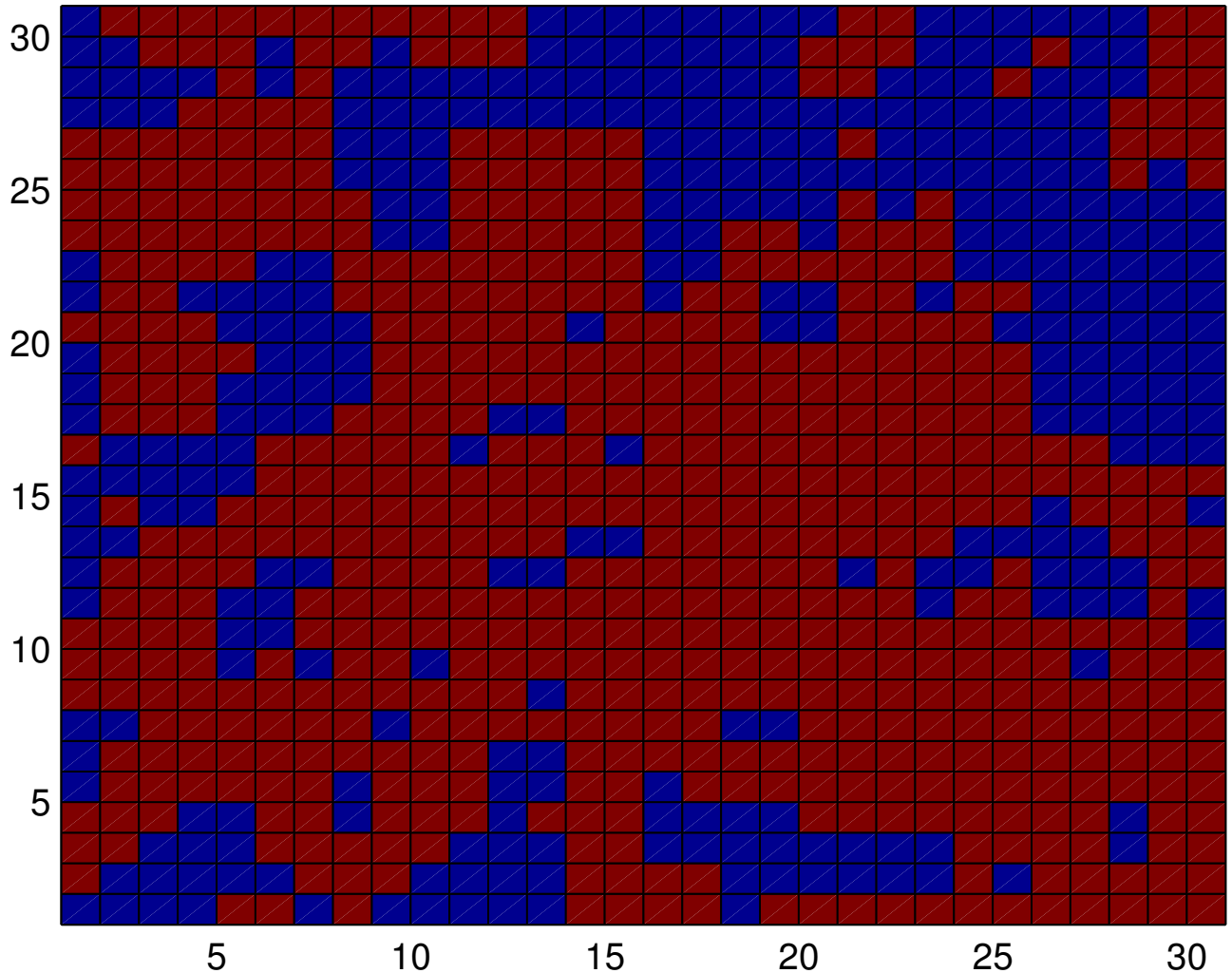

Figure: $T = 2.5$

Visualization of MMC

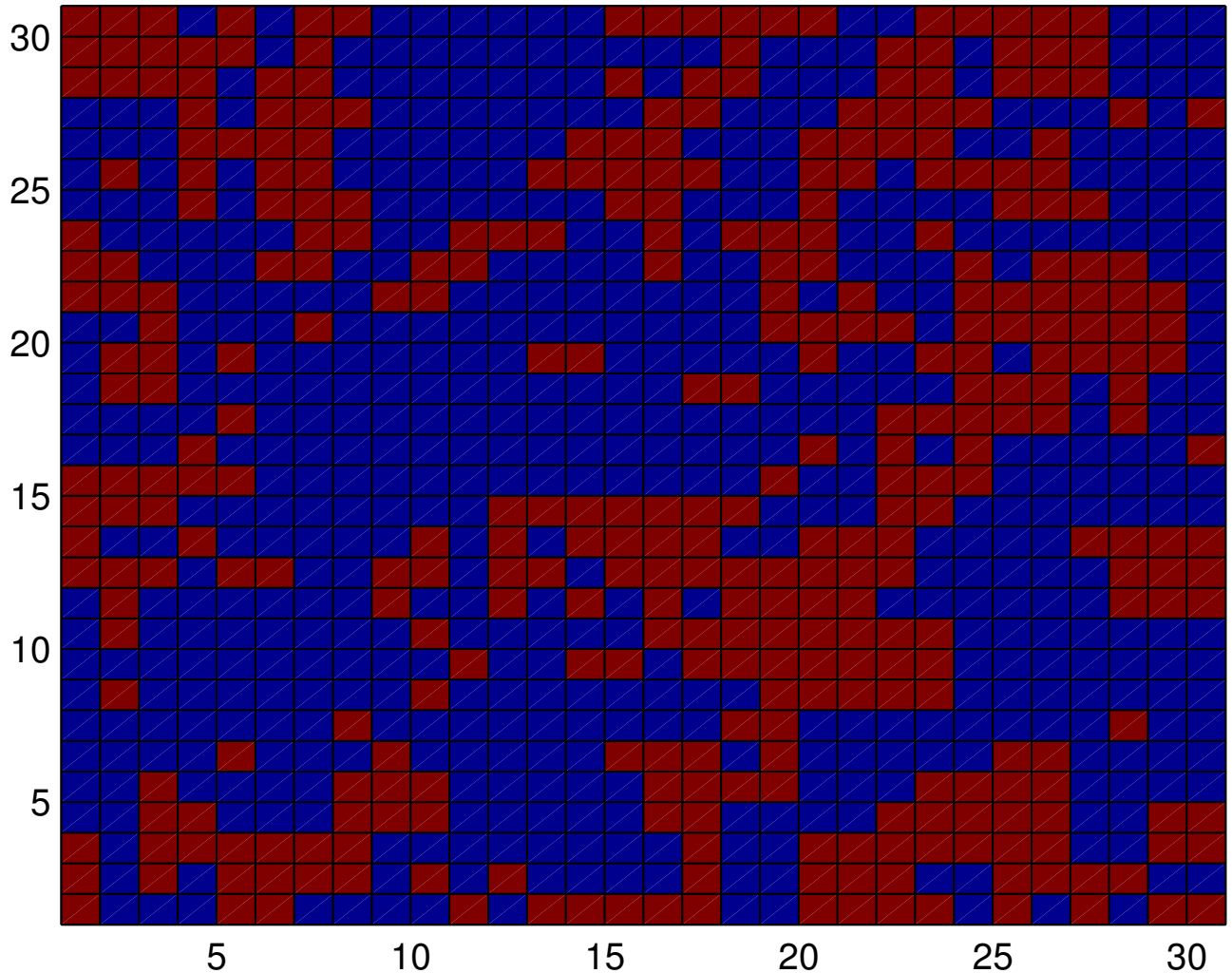

Figure: $T = 3$

Visualization of MMC

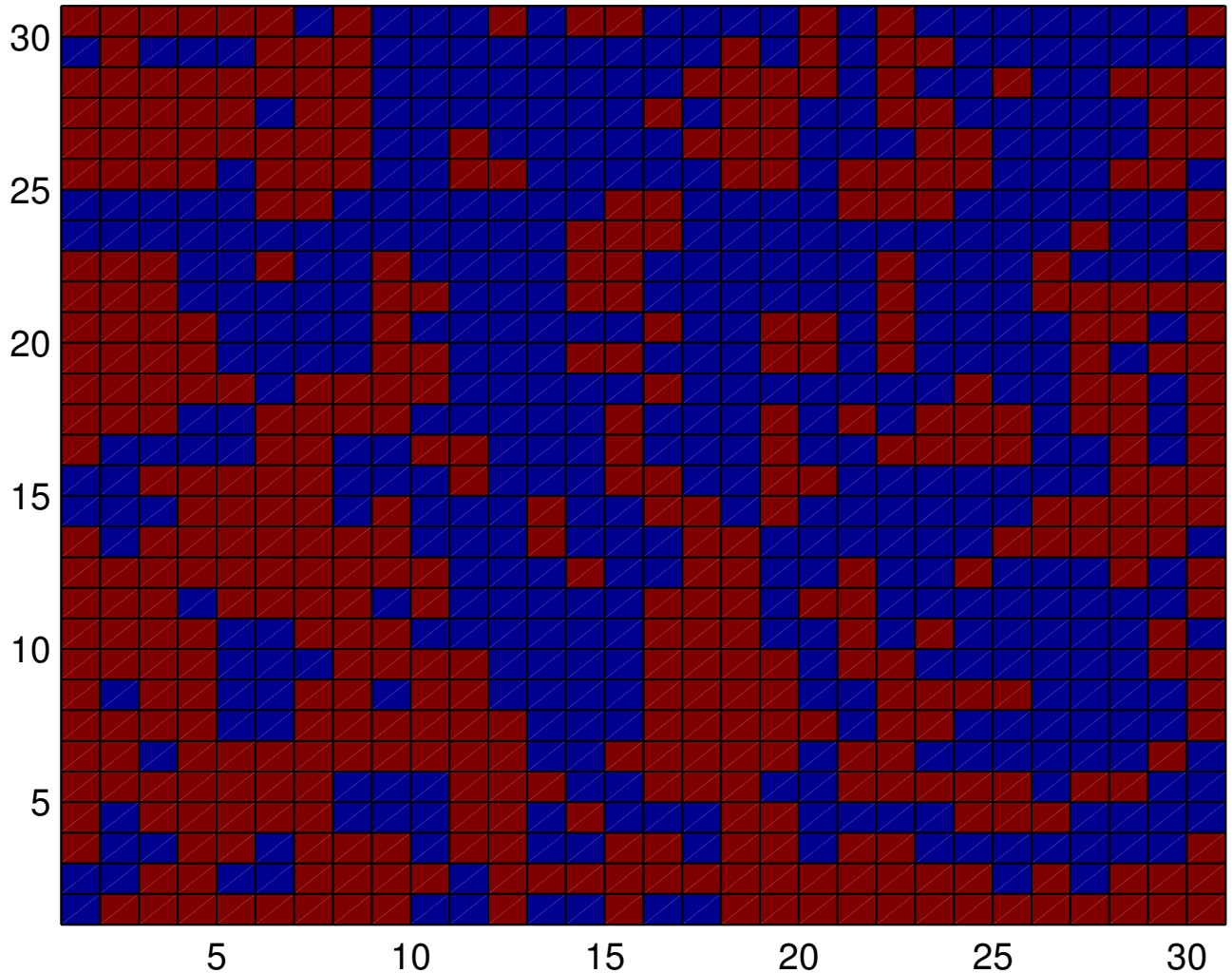

Figure: $T = 3.5$

Visualization of MMC

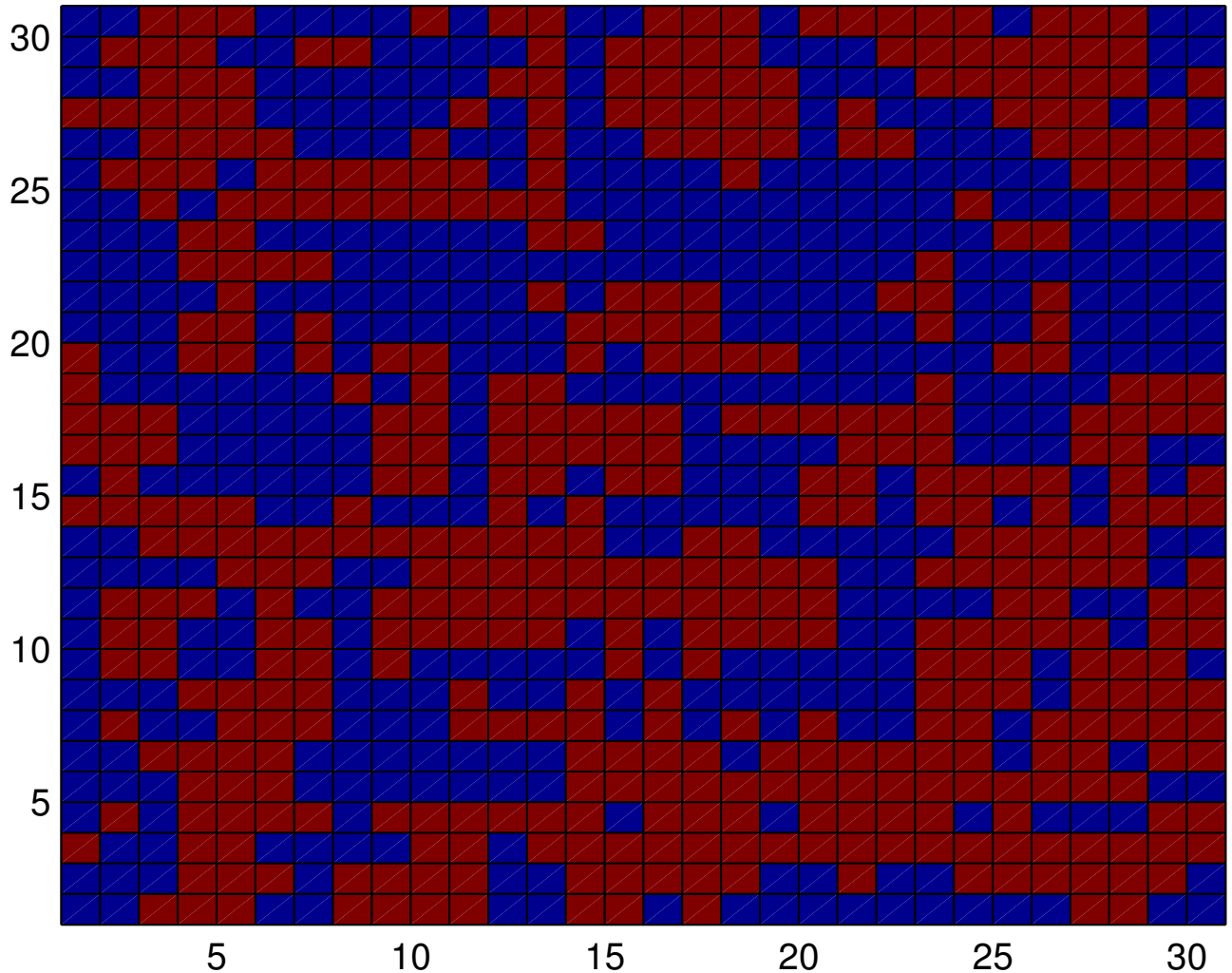

Figure: $T = 4$

Results

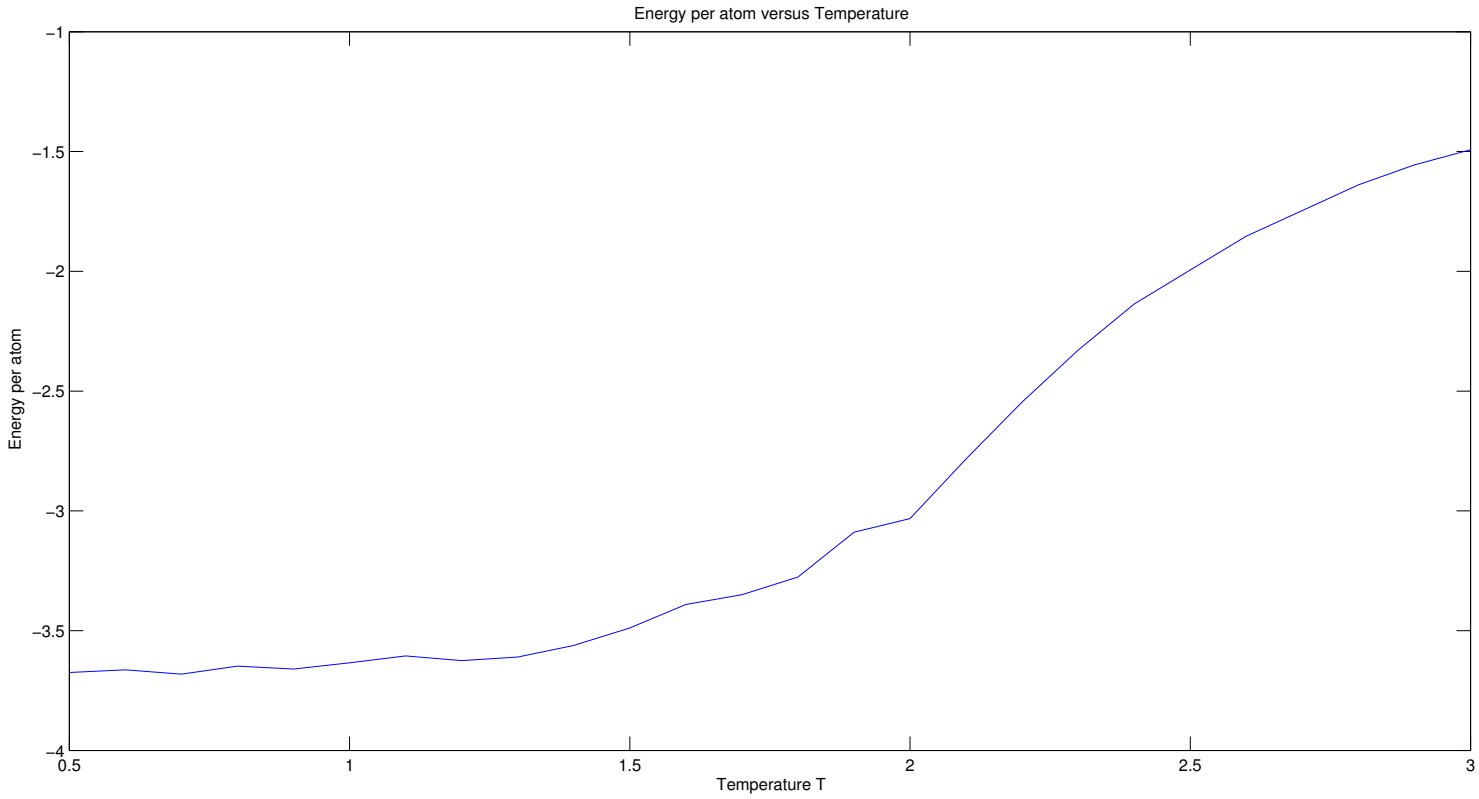

Figure: Energy per site versus Temperature

Results

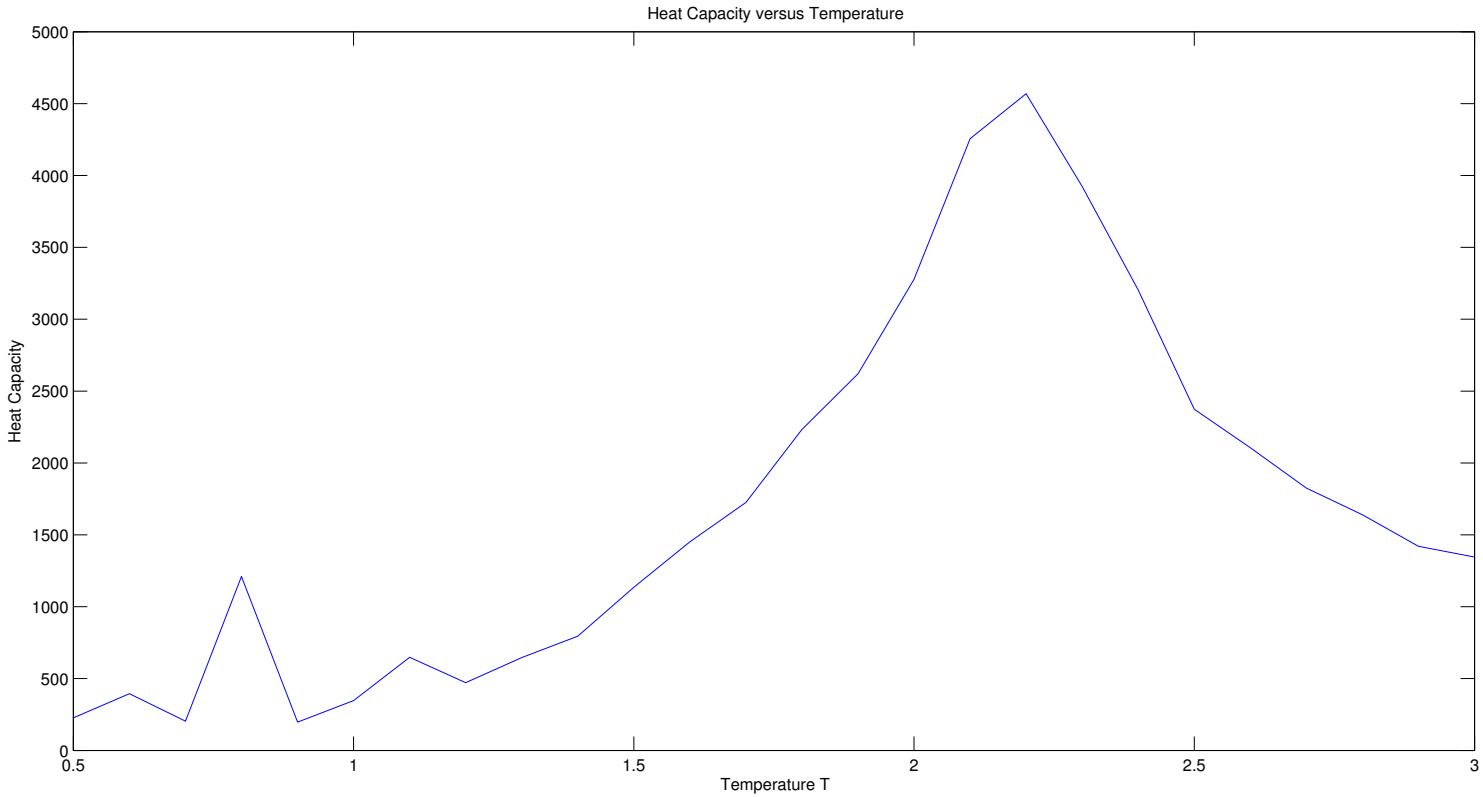

Figure: Heat Capacity versus Temperature

Results

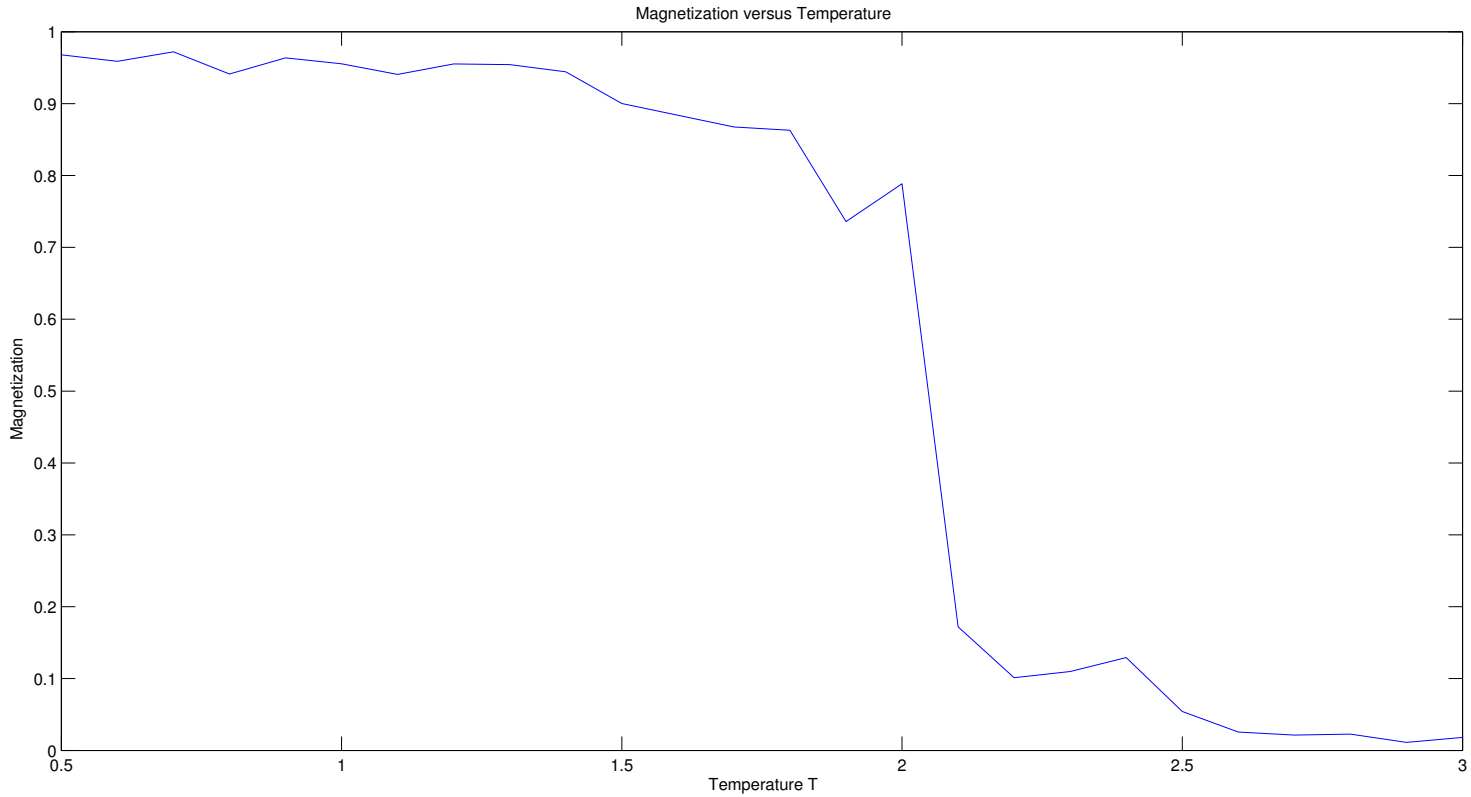

Figure: Magnetization per site versus Temperature

Results

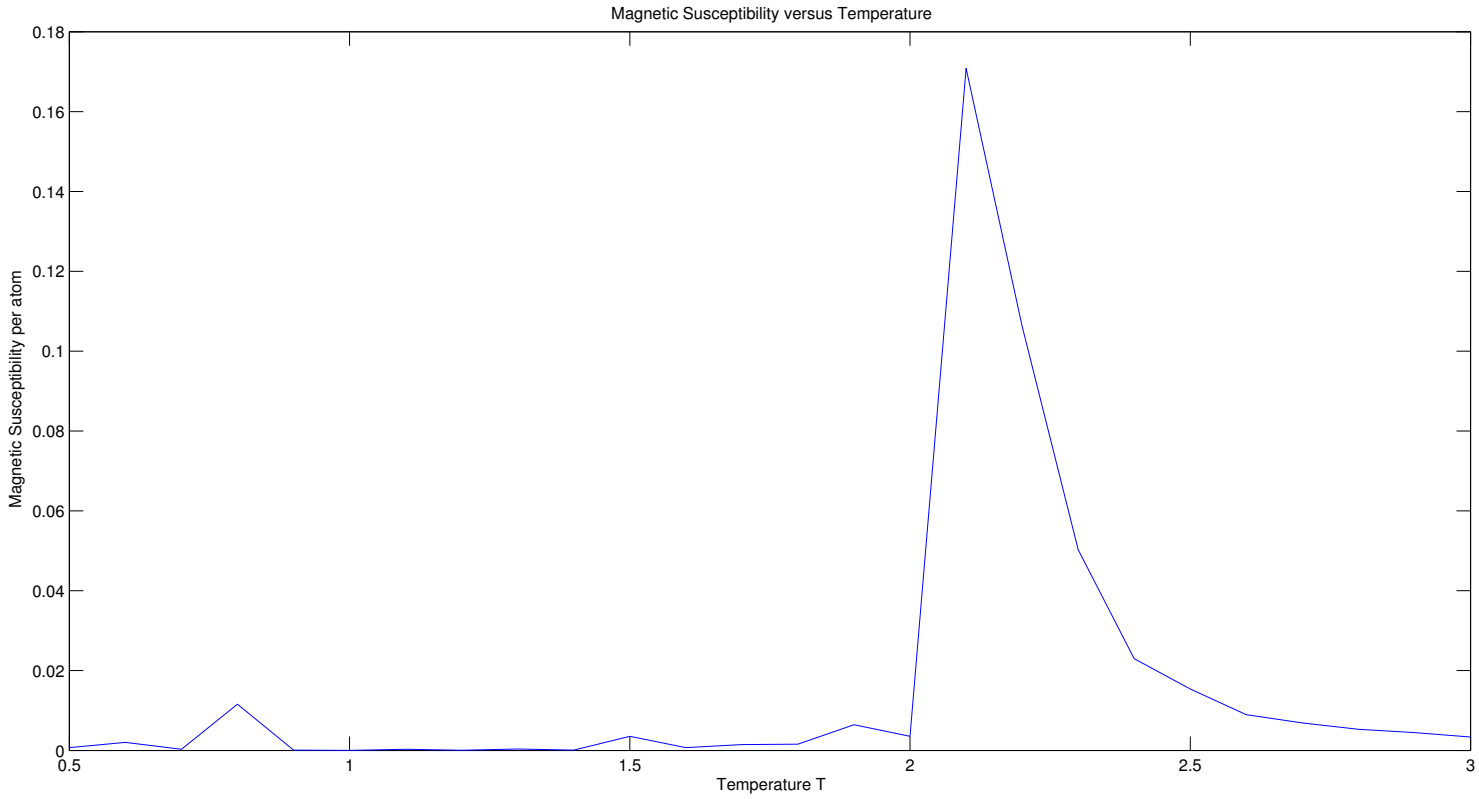

Figure: Magnetic Susceptibility per site versus Temperature

Ehrenfëst Classification of Phase Transitions

- For an n^{th} order phase transition, at the transition point all the n^{th} order derivatives of the ensemble property diverge
- In the Ising model, both specific heat (C_v) and magnetic susceptibility (χ_T) have sharp discontinuites at the Curie temperature
- Since, C_v and χ_T are second order derivatives of ensemble properties, this is classified as a second order phase transition

Physical understanding of the Phase Transition

- As the temperature increases, the tendency to stay ordered reduces because of thermal fluctuations
- The net magnetization, which is a function of net order in the system starts dropping
- Beyond the curie temperature T_c , there is no more tendency to stay ordered, and due to complete disorderness, the net magnetization per site drops to zero

Hysterisis

- The equilibriation is acheived with some value of $h = I$ using the aforementioned algorithm
- Now h is slowly changed to $h = -I$ in discrete steps
- During each of these steps, the previous equilibriated configuration is given as input to the system to undergo equilibriation again
- Average and variance quantities are calculated and plotted

Results

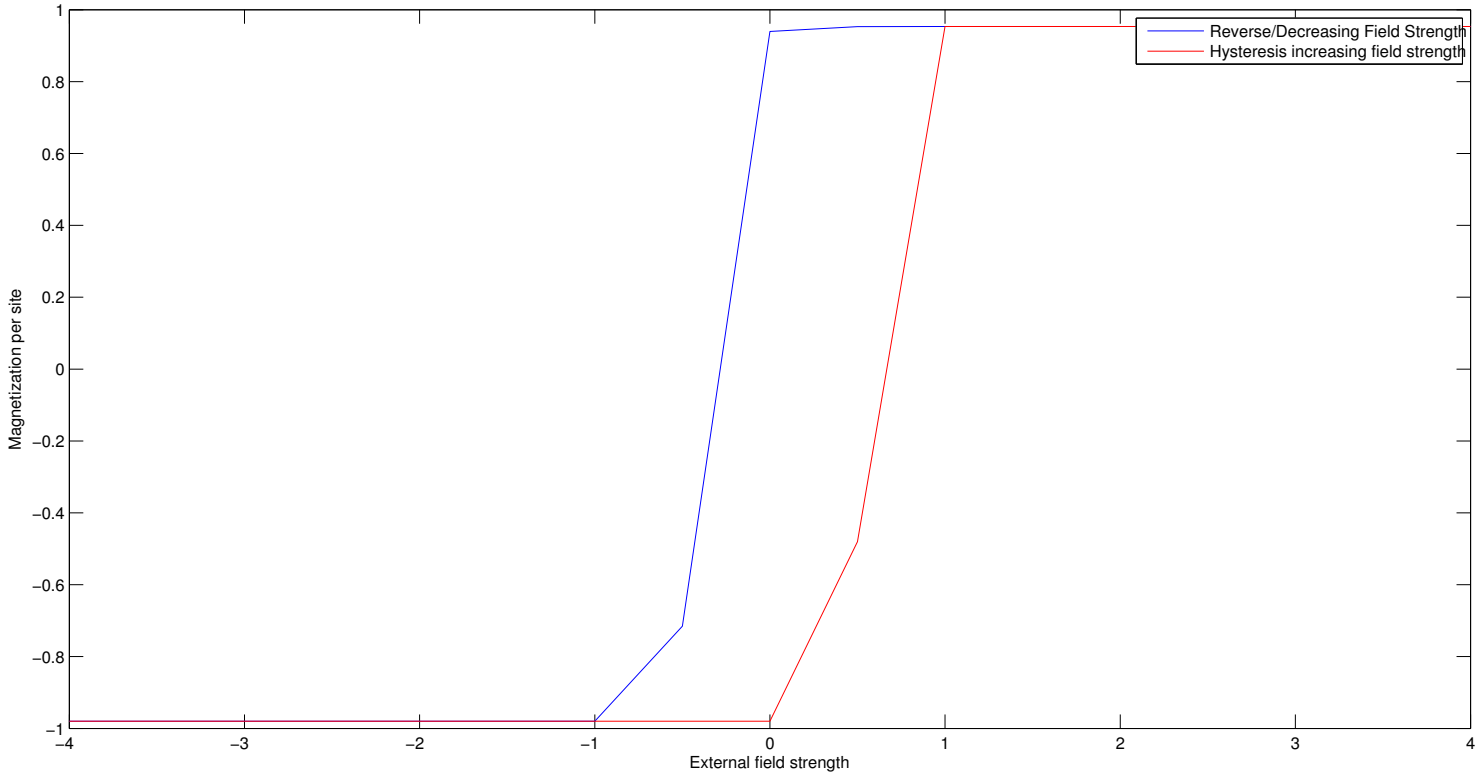

Figure: Hysteresis Loop

Critical Exponents

- Critical exponents describe the behaviour of physical quantities near continuous phase transitions
- It is widely believed, but not proved formally, that these exponents are independent of the physical properties of the system at consideration
- These only depend on the following properties
  - Dimension of interaction
  - Range of Interaction
  - Spin Dimension

Critical Exponents

- Near the phase transition temperature T_C, we define the reduced Temperature $\tau = (T - T_c)/T_c$
- It is stipulated that properties of the system, f_i vary in a power law order, i.e., $f \propto \tau^{\gamma}$, asymptotically as $\tau \to 0$
- Some fluctuations are only observed in one phase, i.e. ordered or disordered
- The difference in the phases is determined by the order parameter ψ, which is Magnetization for Ferromagnetic materials

Critical Exponents

- Some important critical exponents are defined for $C_V \propto \tau^{-\alpha}$, $\psi \propto (-\tau)^{\beta}$ and $\chi_T \propto \tau^{-\gamma}$
- These are estimated from the simulations performed through Partial Least Squares Regression Technique(*of* the log values)

	Analytical	Simulation (MMC)
α	0	0.013
β	$1/8$	0.1288
γ	$7/4$	1.81

Table: Comparison of Analytical and Simulation based Critical Exponents

Anti-Ferromagnetic Materials

- For, anti-ferro magnetic materials, the coupling parameter $J < 0$ between spins.
- This ensures that all the spins are always oppositely aligned at T $<$ Tc,as this maximizes the energy(*From* the Hamiltonian) of the system.
- Since it is symmetric with all other respects(except Magnetization), all the variation in ensemble properties resemble those of the ferromagnetic system
- At temperatures beyond $T > T_C$, the thermal fluctuations start to weigh in and the tendency to remain ordered is removed

Anti-Ferromagnetic Materials

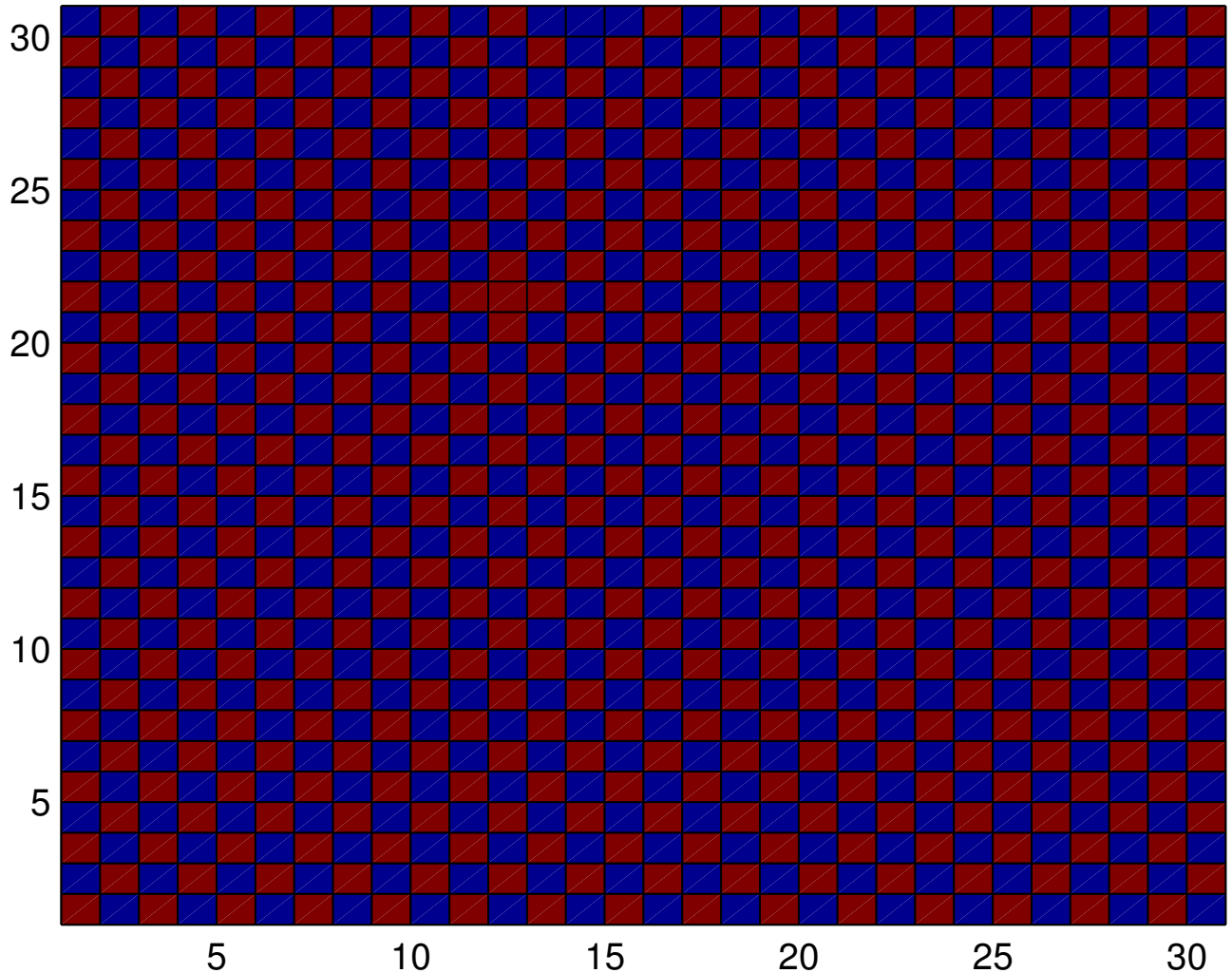

Figure: $T = 1$

Anti-Ferromagnetic Materials

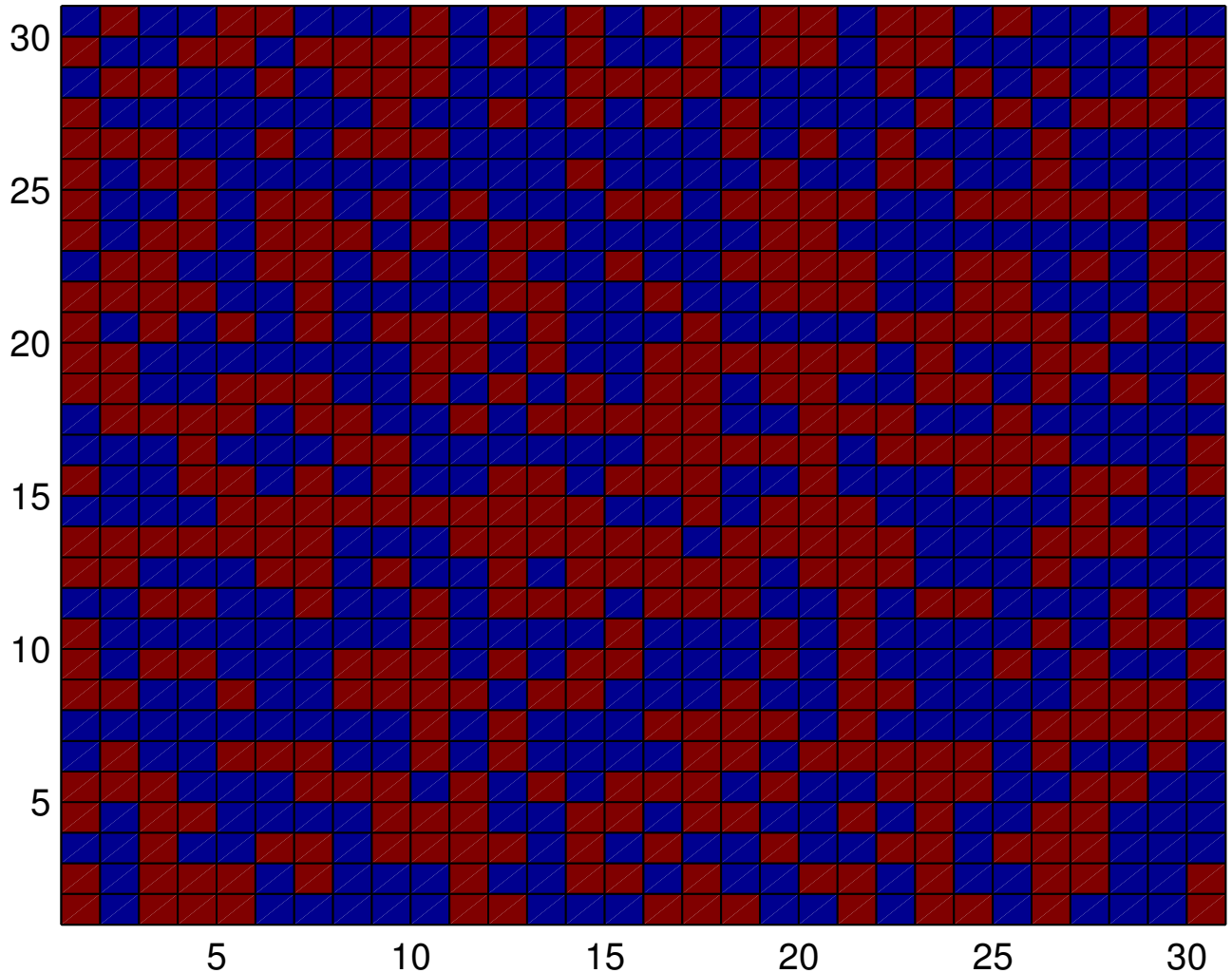

Figure: $T = 3$

Anti-Ferromagnetic Materials

- Antiferromagnetic materials always prefer neighbouring atoms to have alternating spins. Hence presence of external field does not impose any kind of magnetization on the material. This is observed from the simulations that the Net Magnetization Per Atom M, is invariant under external fields
- Since there is no external way to magnetize the system and a state having zero net magnetization is preferred, these kind of materials do not show any cyclic properties or hysteresis loops.

Conclusions

- Phase transition is observed and signified by the change in the order parameter(ψ)/net magentization(M) with increasing temperature in the absence of any external field
- Phase transition is observed (ordered to disordered state) at the curie Temperature of Tc $\approx$ 2.26, in agreement with the analytical result.
- This phase transition is characterized as a second order phase transition based on the divergence/discontinuity characteristic of the second derivative properties, for example Magnetic Suscpetibility χ_T and Constant Volume Heat Capacity C_v .

Conclusions

- The efficacy of Metropolis Monte Carlo Algorithms is evinced by the rapid convergence to equilibrium, taking only a few minutes on a personal computer
- The ability of the algorithm to predict equilibrium values with great precision is very evident in the close overlap between the theoretical and simulation based results of the values of the critical exponents
- An important aspect of ferromagnetic materials, memory of past configurations while subjected to varying external fields(hysteresis) is evinced by these simulations
- In addition, antiferromagnetic systems were also studied and characterized

Possible Extensions to this Work?

- Working with a different force coupling parameter J_{ij} which is distance dependent (Like Lennard-Jones potential)
- Simulating a $3-D$ Ising model and deducing Phase transition properties and critical exponents in $3-D$
- Extrapolating the Ising Model to a Lattice based Gas Model and predicting phase transition based on revised order parameter $\psi = \frac{\rho - \rho_c}{\rho_c}$
- Try and establish validity of Ising model for alloys/mixtures of ferromagnetic substances and predicting phase transition phenomena

References

- Onsager, Lars (1944), "Crystal statistics. I. A two-dimensional model with an order-disorder transition", Phys. Rev. (2) 65 (3–4): 117–149
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- Markov Processes, Gillespie, 4^{th}edn
- Class Notes!