3D Ising Model with Swendsen Wang Cluster Update

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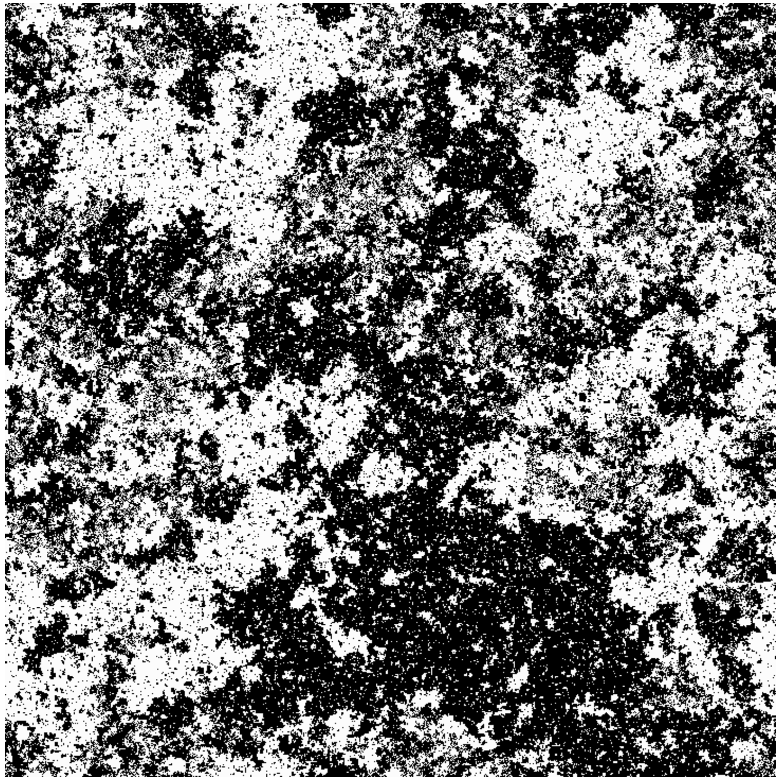

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Ising Model: Introduction

- Ising Model is one of the most well studied models in statistical mechanics
- Simple dynamics lead to complex emergent behavior
- 1D model solved by Ising in 1925
- 2D model solved in 1944 by Onsager

- For D => 3 no exact solution exists

- Perfectly suitable for Simulations

Ising Model: Dynamics

- Ising model defined by the Hamiltonian

$$H(\sigma) = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j$$

- Goal
  - Simulate 3D Ising Model on a lattice
  - Verify a phase transition occurs and extract the critical temperature, T_c
  - Extract the critical exponents describing the behavior of thermodynamic variables near T_c

Algorithm

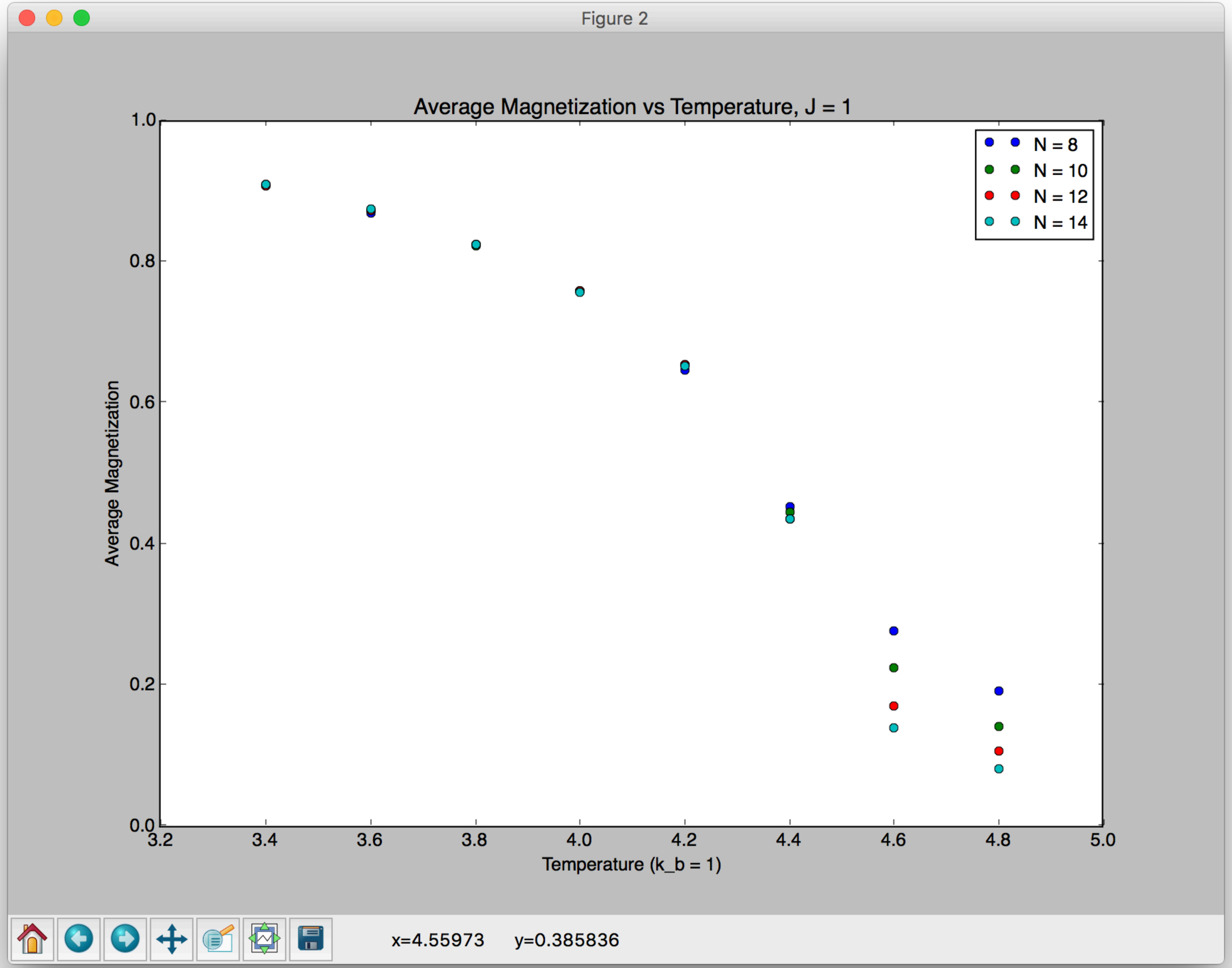
- On our homework we utilized a single spin flip Metropolis algorithm
  - Update spin configuration by flipping a single spin and calculating the change in the total energy
  - Suffers from critical slowing down

- Solution posed by Swendsen and Wang
  - Add additional degree of freedom (bonds)
    - two neighboring spins can be disconnected, or connected
    - If they point in opposite directions, they are disconnected
    - If they point in the same direction, they are connected with probability $1 - \exp(-2\beta J)$
    - Hoshen-Kopelman algorithm identifies clusters of connected spins
    - Perform thermodynamic measurements
    - Flip each cluster of spins with probability 1/2

Measurements

- Simulated the 3D Ising model for lattice sizes of 8,10,12,14 over a range of temperatures ($3k_b$ to $5k_b$)
- 1000 steps to equilibrate the system and an additional 4000 measurements at each temperature
- Extracted m (magnetization/site), χ (susceptibility), C_v (heat capacity)

Magnetization



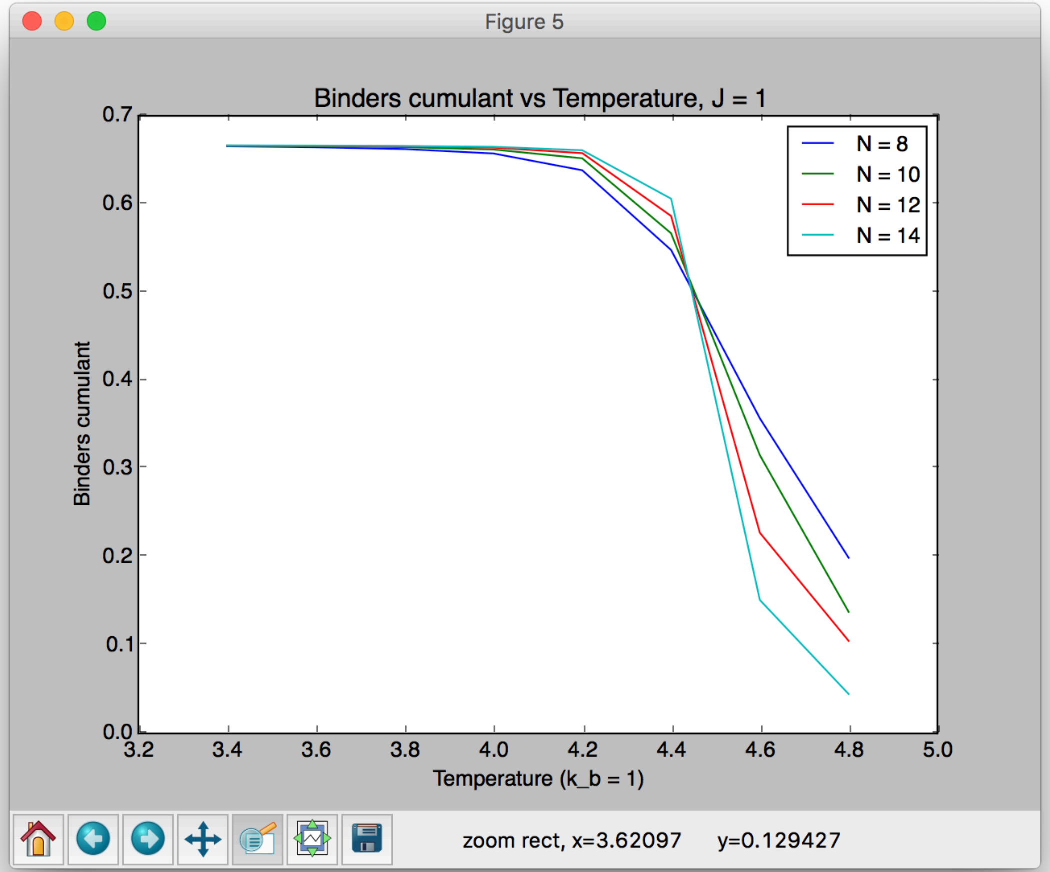
Binder's Cumulant

- Cumulant defined as $U = 1 - \frac{\langle M^4 \rangle}{3\langle M^2 \rangle^2}$

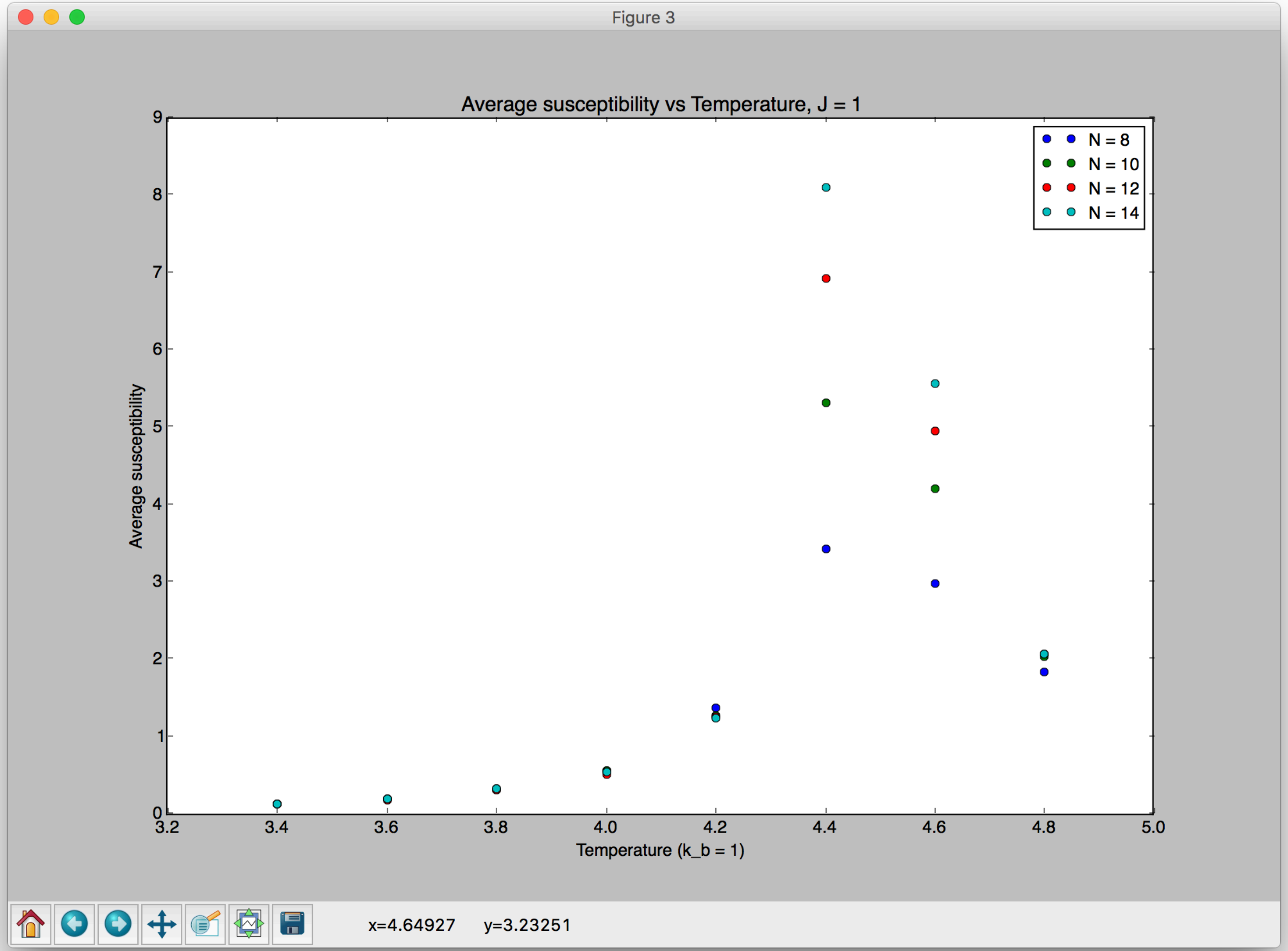
- Finite size scaling tells us the binder cumulant obtains a universal value at T = T_c regardless of system size

- By plotting it for different system sizes and looking for the common intersection, we can obtain a good estimate of the critical temperature

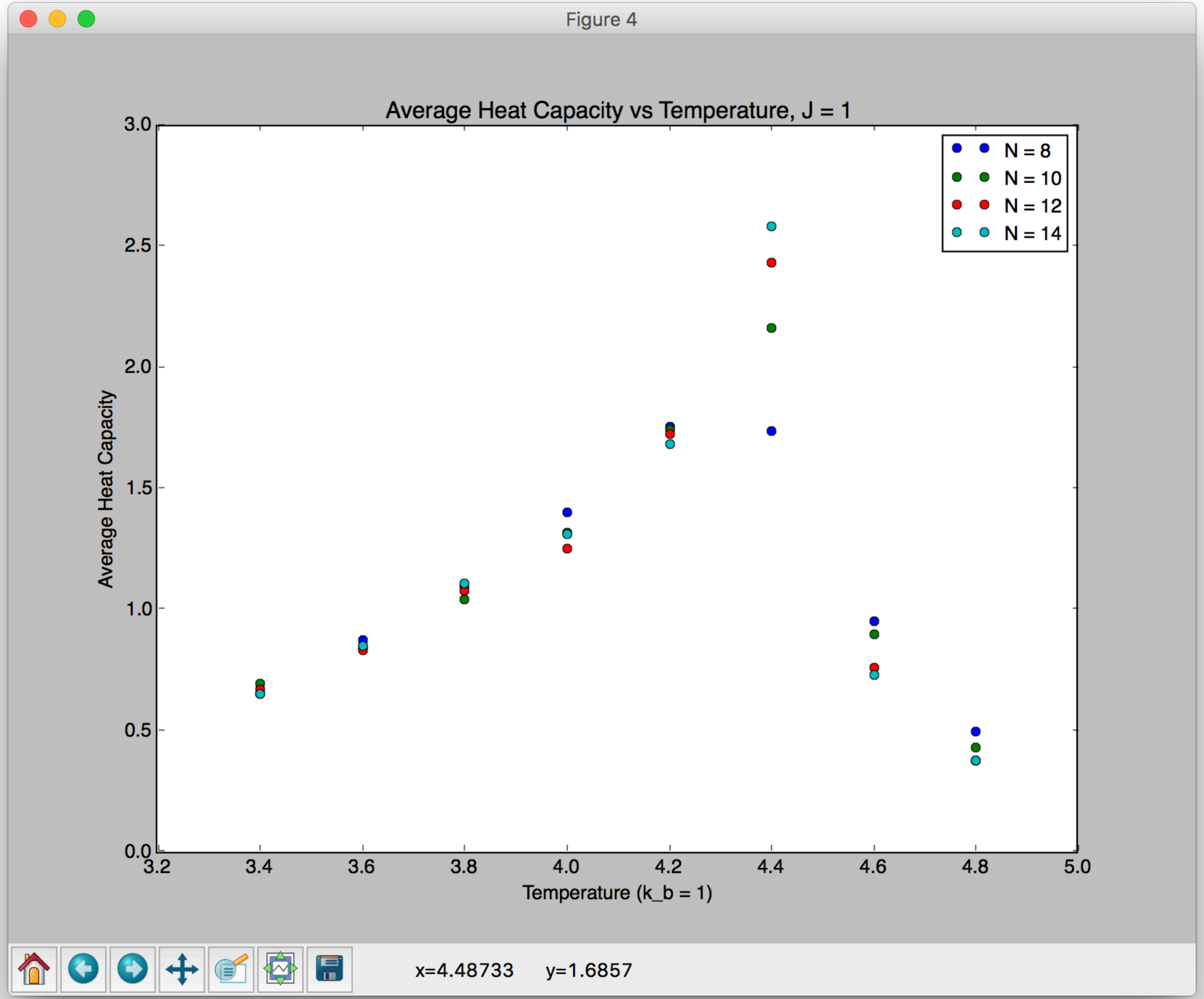
- Estimated T_c from these simulations is ~4.45



Susceptibility



Heat Capacity



Critical exponents

- The critical exponents describe the behavior of the system near criticality
  - Power law behavior

$$M(T) \sim (T_c - T)^{\beta}$$
$$C \sim |T - T_c|^{-\alpha}$$
$$\chi \sim |T - T_c|^{-\gamma}$$

  - We can use finite size scaling analysis to turn these relationships between our thermodynamic variables and the lattice size

$$|T - T_c(L)| \approx L^{\frac{-1}{\nu}}$$

  - Then

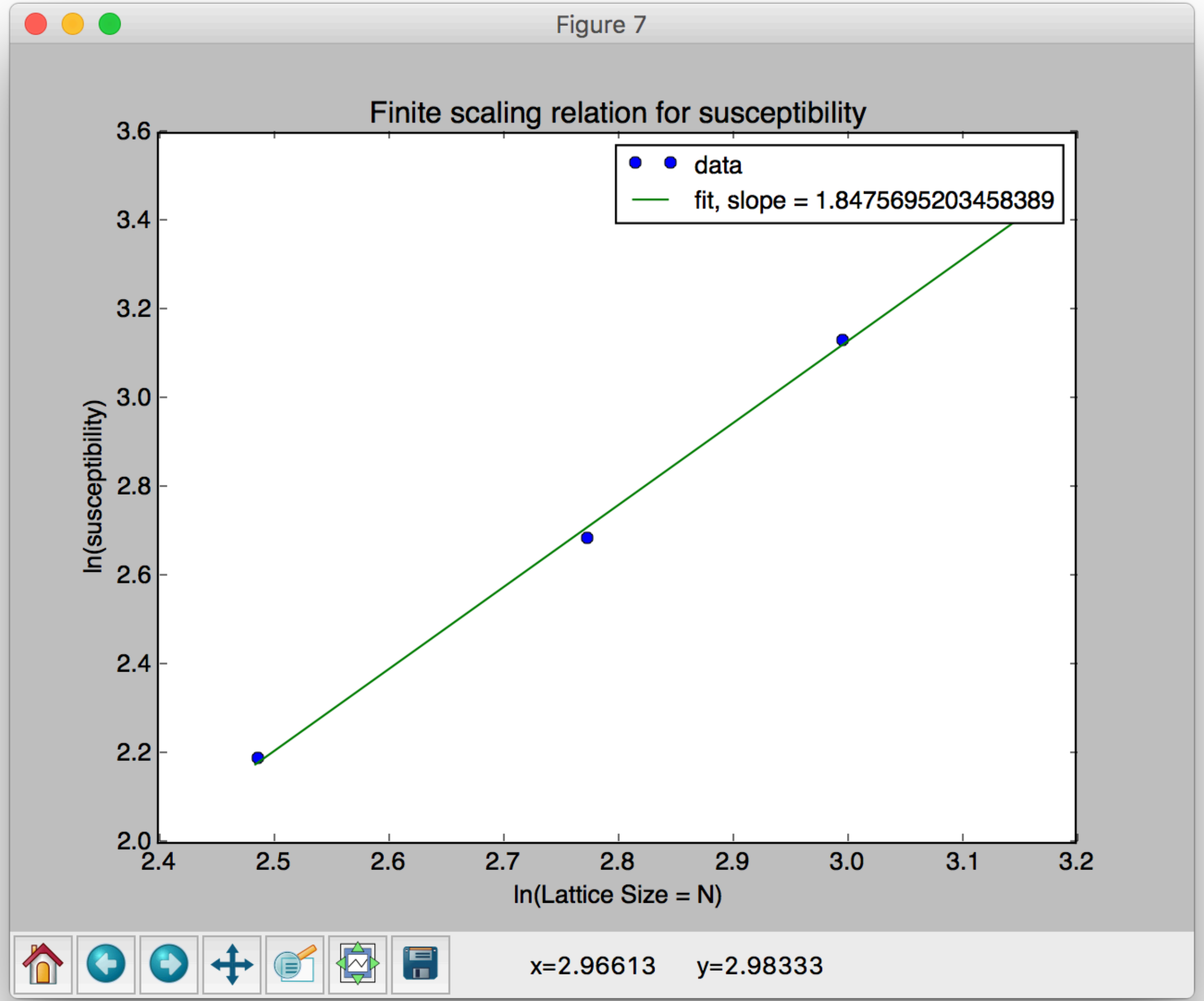
$$M \approx L^{-\frac{\beta}{\nu}}$$
$$C \approx L^{\frac{\alpha}{\nu}}$$
$$\chi \approx L^{\frac{\gamma}{\nu}}$$

Critical exponents

- We can then extract the critical exponents by plotting the logarithm of our thermodynamic variables vs. the logarithm of the system size
- We fit our data and can then extract the critical exponents as the slope of the fit
- Note: Did not obtain the critical exponent for the correlation length so we use the accepted value $\nu = .63$

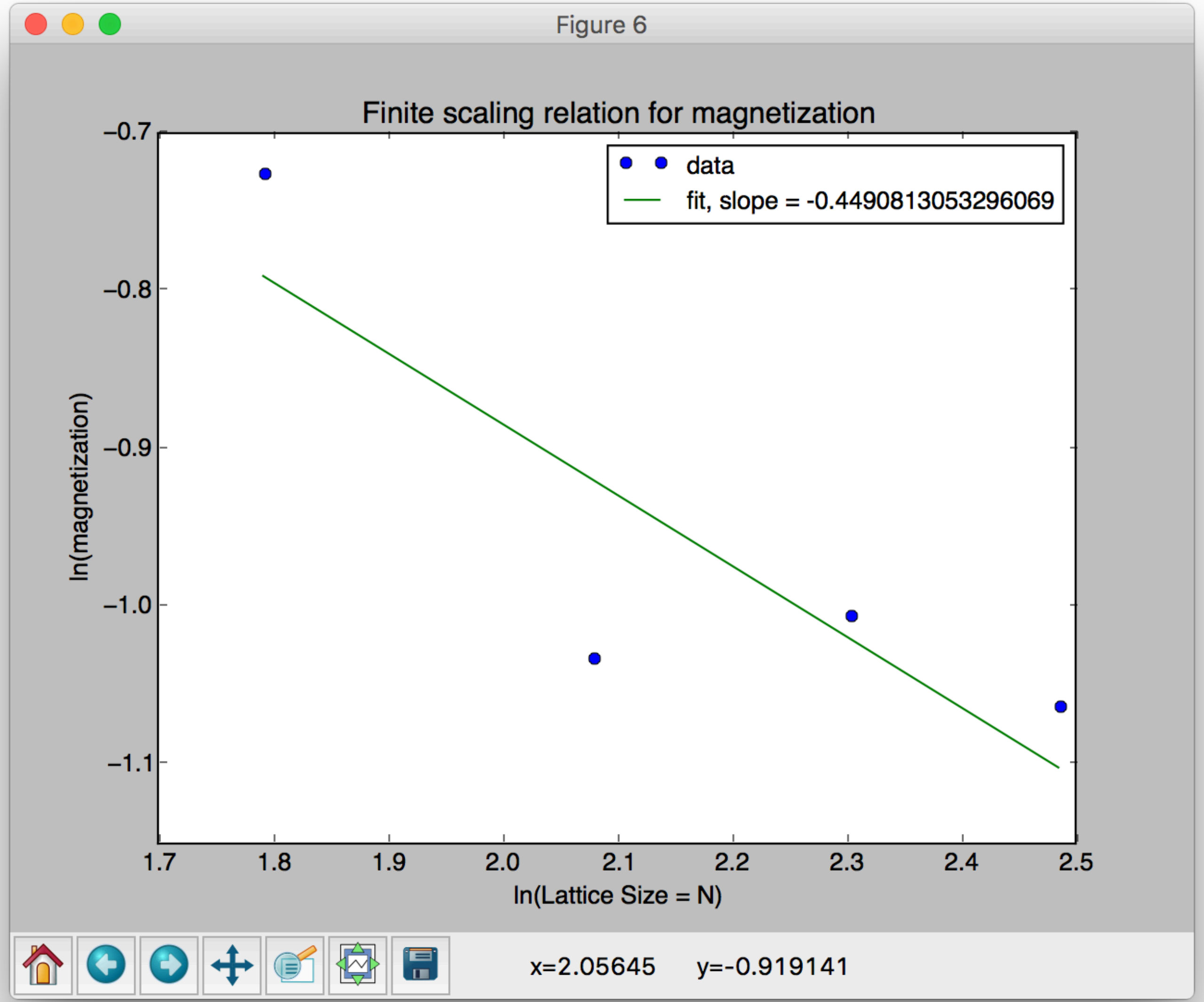
Critical exponents

- Theoretical value = 1.96



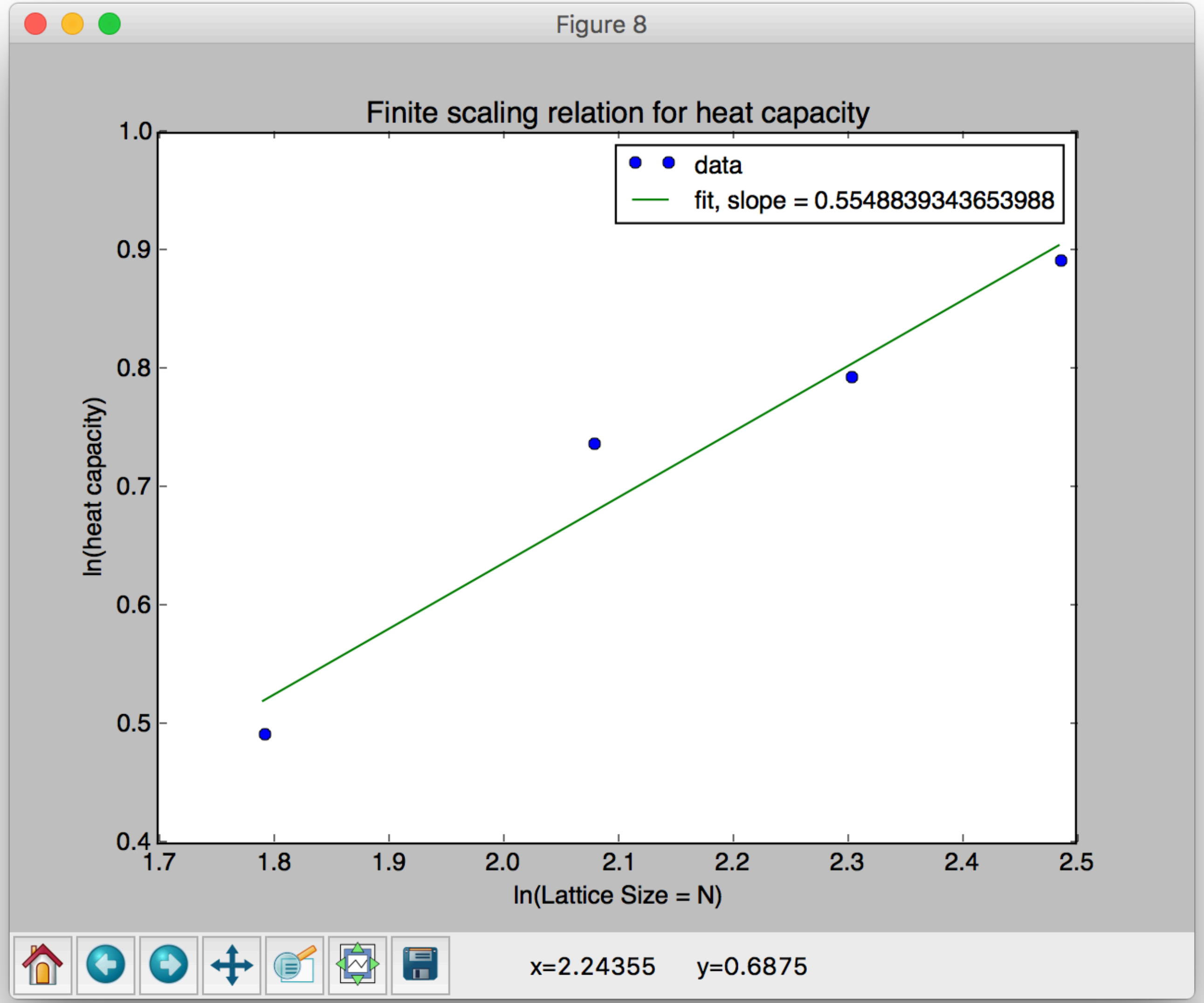
Critical exponents

- Theoretical value = .52



Critical exponents

- Theoretical value = .17



Conclusion

- We simulated the 3D ising model using the Swendsen Wang Update
- Observed a phase transition at $T_c = 4.45k_b$
- Extracted critical exponents of describing the behavior of the system near criticality