2D Ising Model

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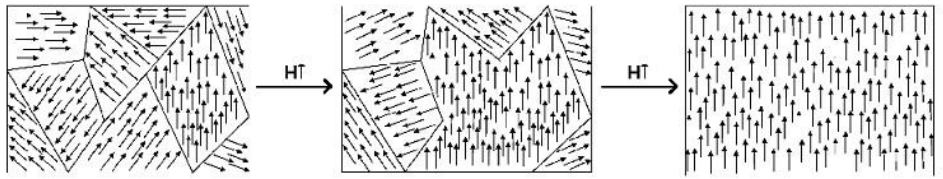
Outline

- Introduction to Ferromagnetism and the Ising Model
- Monte Carlo Methods and the Metropolis Algorithm
- Implementation
- Tests of Code
- Results
  - Equilibrium time
  - Probability Distributions
  - Phase Transitions
- Conclusions

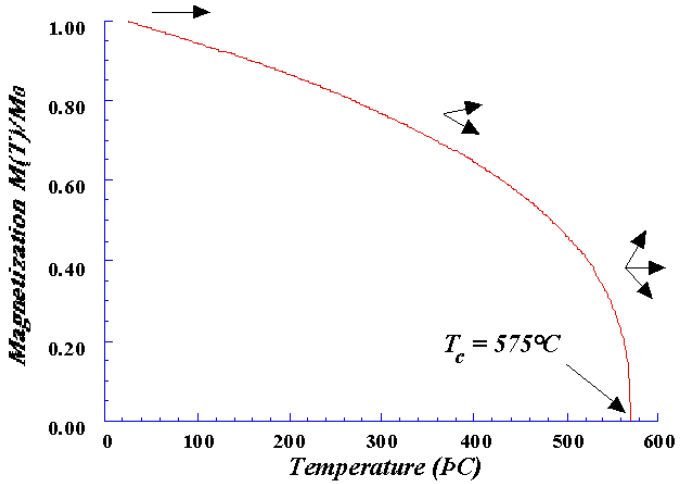
Ferromagnetic Materials

- Materials that exhibit domains where the spins of unpaired electrons align
- Domains grow with an applied B field and can be maintained after the B field is removed



http://pediaa.com/

- This alignment competes with thermal excitations
- At the Curie temperature, spins are forced out of alignment
  - Phase Transition



http://www.irm.umn.edu/hg2m/hg2m_b/hg2m_b.html

The 2D Ising Model

- Models spins on two dimensional lattice where closest neighbors interact

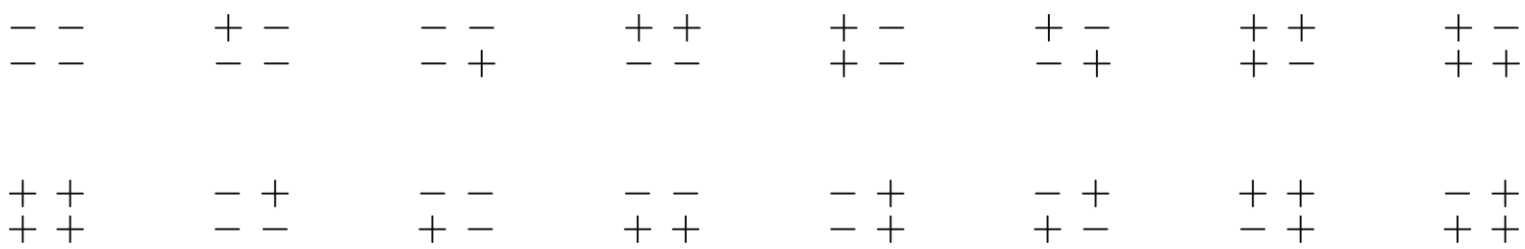
$$E = -J \sum_{\langle kl \rangle}^{N} s_k s_l .$$

- Very simple model that allows us to study properties of phase transitions

- Has been widely applied outside of ferromagnetism
  - Anti-ferromagnetism
  - Opinions on the economy
  - Urban segregation
  - Language evolution

Staugger, D. Applications of two-dimensional Ising Models. arXiv: 0706.3983

2 by 2 Lattice with Ising Model



Number of Spin Ups	Number of Configurations	Energy	Magnetization
0	1	-8J	-4
1	4	0	-2
2	4	0	0
2	2	8J	0
3	4	0	2
4	1	-8J	4

2 by 2 Lattice with Ising Model

- Because of the limited number of energy states, we can calculation the partition function explicitly

$$Z = \sum_{i=1}^{M} e^{-\beta E_i}$$

- Expectation values can be calculated using the formula

$$\langle X \rangle = \sum_{i=1}^{M} X_i P_i \qquad \text{where} \qquad P_i(\beta) = \frac{e^{i\beta E_i}}{Z}$$

- In this work we examined the behavior of 4 quantities

$$\langle E \rangle = \frac{-8Jsinh(8\beta J)}{3 + cosh(8\beta J)} \qquad \langle |M| \rangle = \frac{2(2 + e^{8J\beta})}{3 + cosh(8\beta J)}$$

$$C_V = \frac{1}{T^2}(\langle E^2 \rangle - \langle E \rangle^2) = \frac{64J^2}{T^2}\frac{1 + 3cosh(8J\beta)}{(3 + cosh(8J\beta))^2} \qquad \chi = \frac{1}{T}(\langle M^2 \rangle - \langle |M| \rangle^2). = \frac{4}{T}\frac{3 + 4cosh(8J\beta) + 2sinh(8J\beta)}{(3 + cosh(8J\beta))^2}.$$

Introduction to Monte Carlo

- Monte Carlo Methods are statistical simulation methods
  - Use random numbers to preform simulation
- Useful in situations where the behavior of a system cannot be easily described analytically

- The general components of a Monte Carlo method are
  - A PDF which characterizes a system
  - Calculation of random numbers to create proposed transition in the system
  - A sampling rule to decide whether or not to accept a proposed transition

$$P_i(\beta) = \frac{e^{i\beta E_i}}{Z}$$

$$Z = \sum_{i=1}^{M} e^{-\beta E_i}$$

The Metropolis Algorithm

- The PDF for large (physical) systems is intractable and we don't know the transition probability analytically
  - Make a choice for the transition probability, W

$$w_i(t+1) = \sum_j W_{ij} w_j(t) \qquad W(j \to i) = T(j \to i) A(j \to i)$$

- Then we can write the full expression

$$w_i(t+1) = \sum_j [w_j(t) T_{j \to i} A_{j \to i} + w_i(t) T_{i \to j} (1 - A_{i \to j})]$$

- Simplify using normalization of probabilities, equilibrium conditions, and detailed balance

Hjorth-Jensen, Morten. Computational Physics, Lecture Notes Fall 2015.

The Metropolis Algorithm

- Then we are left with

$$\frac{A(j \to i)}{A(i \to j)} = e^{-\beta(E_i - E_j)}.$$

- The Metropolis Algorithm is the sampling rule that we get from this relation

$$A(j \to i) = \begin{cases} e^{-\beta(E_i - E_j)} & \text{if } E_i - E_j > 0 \\ 1 & \text{else} \end{cases}$$

- Accept all transitions to a lower energy state. Transitions to higher energy states are accepted with some probability depending on change in energy
  - Preserves ergodicity

Hjorth-Jensen, Morten. Computational Physics, Lecture Notes Fall 2015.

Implementation

```
subroutine Metropolis(NumSpins, idum, SpinMatrix, E, M, w)
  implicit none

  integer::NumSpins,x,y,ix,iy,deltaE,right,left,up,down,idum
  integer, dimension(NumSpins,NumSpins)::SpinMatrix
  real(8)::E,M
  real(8)::w(-8:8)
  do y=1,NumSpins
     do x=1,NumSpins
        ix=int(rand()*NumSpins)+1
        iy=int(rand()*NumSpins)+1
        right = ix+1
        if (ix == numspins) then
           right = 1
        end if
        left = ix-1
        if (ix == 1)then
           left = numspins
        end if
        up = iy+1
        if (iy == numspins) then
           up = 1
        end if
        down = iy-1
        if (iy == 1) then
           down = numspins
        end if
        deltae = 2*spinmatrix(ix,iy)*(spinmatrix(right,iy)+&
             spinmatrix(left,iy)+spinmatrix(ix,up)+ &
             spinmatrix(ix,down) )
        if ( rand() <= w(deltae) ) then
           spinmatrix(ix,iy) = -spinmatrix(ix,iy)
           M = M+2*spinmatrix(ix,iy)
           E = E+deltaE
        end if
     end do
  end do
end subroutine Metropolis
```

1) Using a random number generator, choose a random position on the lattice and compute the energy of that state.
2) Flip only one spin in that configuration and compute the new energy of the state.
3) Calculate the energy difference between these two state.
4) If the energy difference is less than 0, we accept the transition.
5) If the energy difference is greater than 0, we calculate $w = e^{-\beta \Delta E}$
6) We generate a random number between 0 and 1. If that number is less that w, we accept the change. If not, we keep the old configuration.
7) Update expectation values for various quantities.
8) Repeat these steps for each desired Monte Carlo iteration at every desired temperature.

Verifying Code with 2 by 2 Lattice

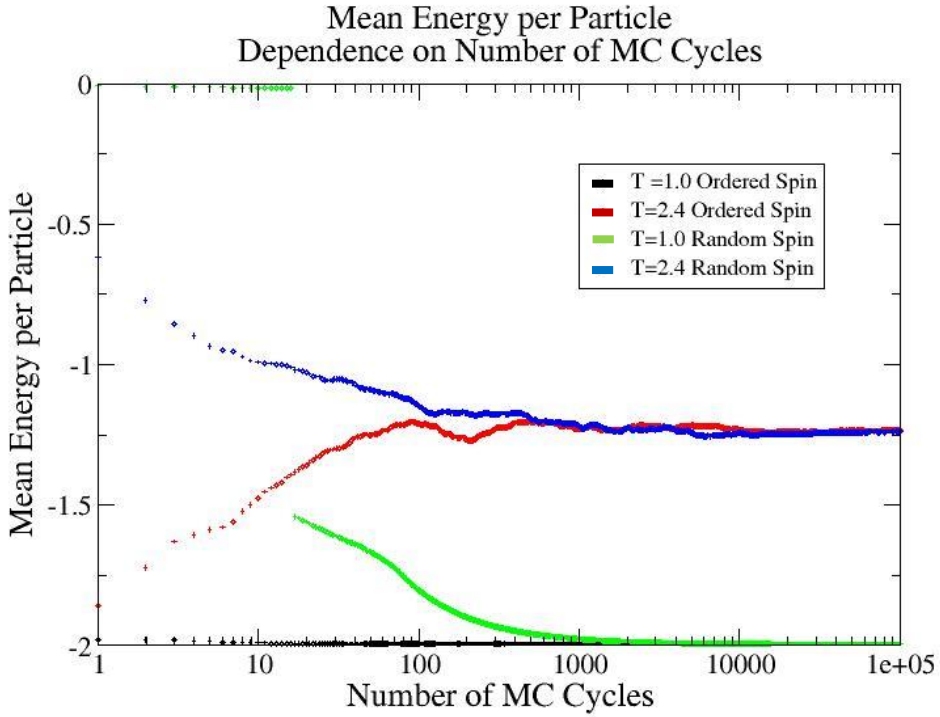
- Ran calculation with T=1.0 (units if kT/J) and compared to exact results

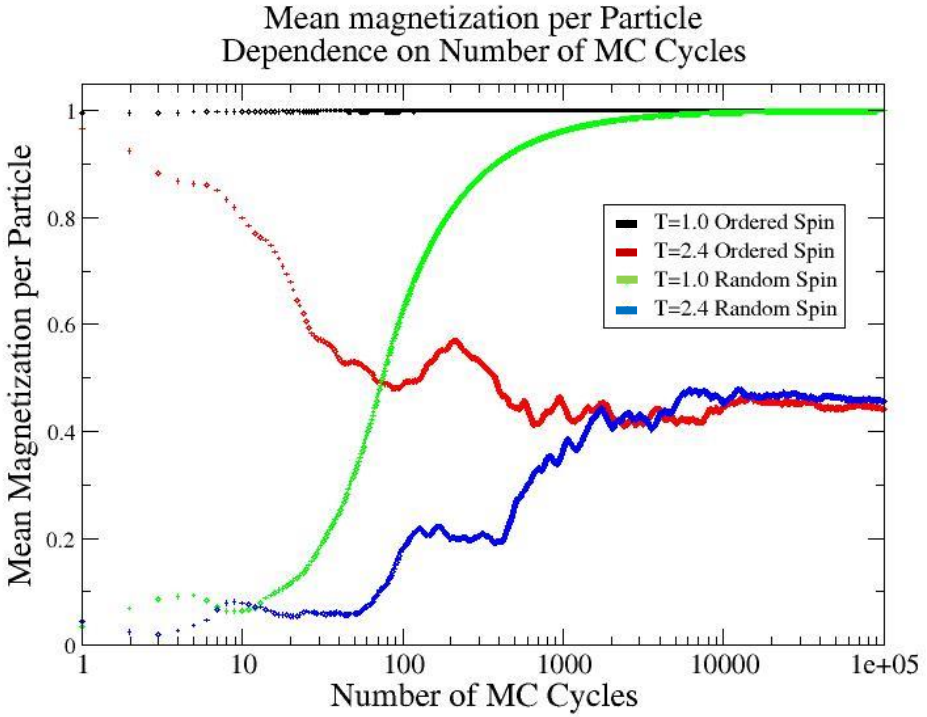
Exact: -1.99598 0.998661 0.0320823 0.00401074

Cycles	E/N	ϵ	$\lvert M\rvert/N$	ϵ	C_V/N	ϵ	χ/N	ϵ
10	-1.8182	0.0891	0.9091	0.0869	1.3223	40.2163	0.3306	81.4232
50	-1.9608	0.0176	0.9894	0.0183	0.3076	8.5870	0.0769	18.1719
100	-1.9208	0.0377	0.9703	0.0284	0.6086	17.9689	0.0955	22.8063
500	-1.9521	0.0290	0.9820	0.0166	0.3741	10.6592	0.0586	13.6080
1000	-1.9740	0.0110	0.9905	0.0082	0.2051	5.3927	0.3061	6.6317
5000	-1.9908	2.5953E-3	0.9966	2.0625E-2	0.0732	1.2831	0.0112	1.7804
10000	-1.9928	1.5939E-3	0.9974	1.3123E-3	0.0574	0.7887	8.6711E-3	1.1620
50000	-1.9945	7.5256E-4	0.9981	5.8151E-4	0.0440	0.3726	5.9893E-3	0.4923
100000	-1.9955	2.6162E-4	0.9985	2.0301E-4	0.0363	0.1305	4.721E-3	0.17697
500000	-1.9961	7.9066E-5	0.9987	4.9233E-5	0.0308	0.0393	3.8735E-3	0.0342
1000000	-1.9961	4.9031E-5	0.9987	2.4270E-5	0.0313	0.0244	3.9692E-3	0.01036

Results – Equilibrium Time

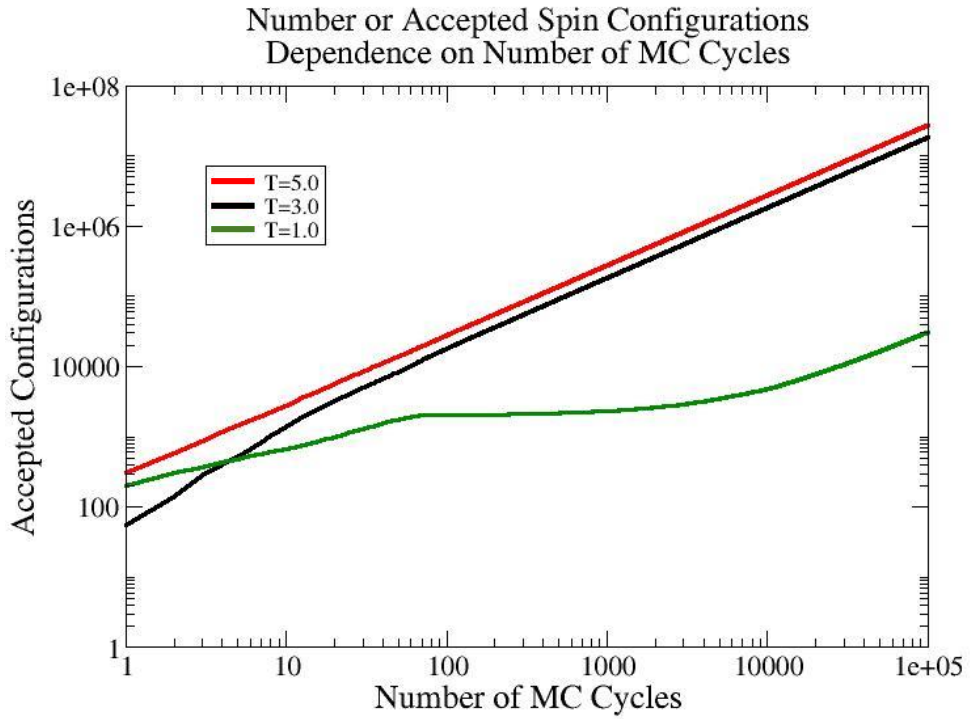
- We can explore how long it takes to reach equilibrium, using MCS as a proxy for time
  - 20 by 20 Lattice at T=1.0 and 2.4 (well below and above critical temperature)





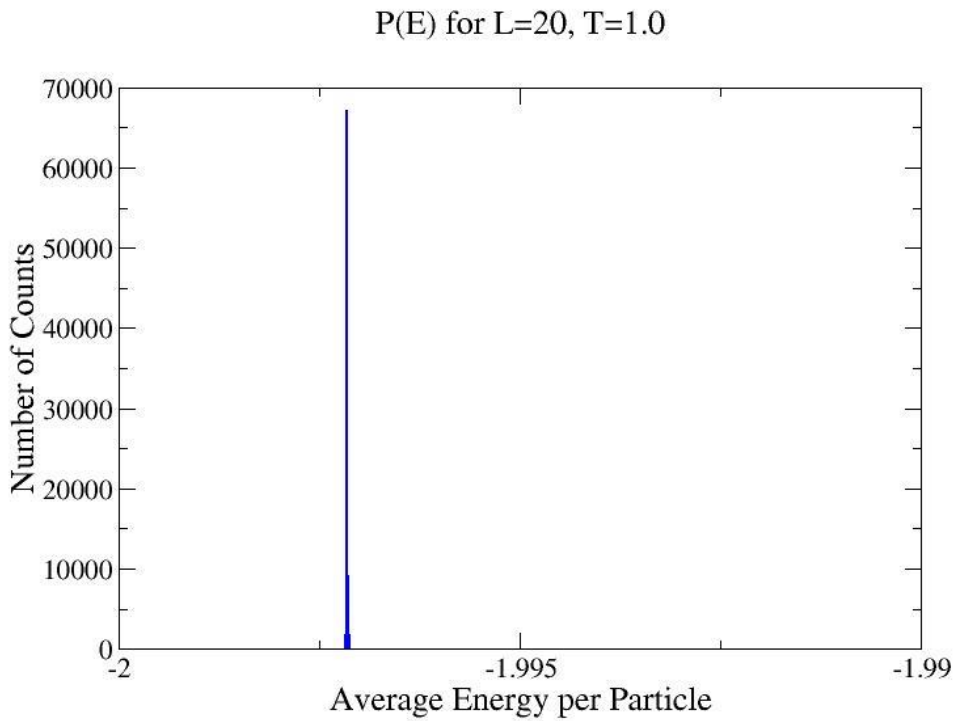
Results – Accepted Transitions

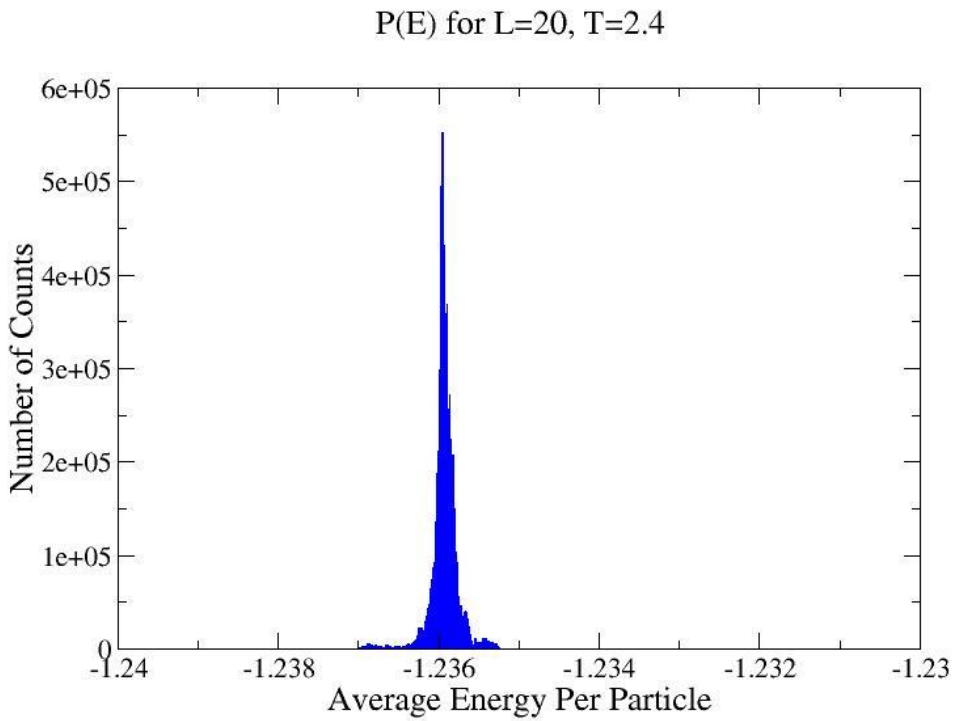
- We can study the number of accepted spin configurations as a function of MCS at different temperatures
- Log-log plot reveal linear relationship
- Slope increases with temperature
- As the temperature increases, more configurations are open to the system, allowing for a higher acceptance



Results – Probability Distributions

- Compare energy probability distribution at T=1.0 and T=2.4
  - Widening of distributions is related to the variance, which is captured by the heat capacity.





Introduction to Phase Transitions

- Near the critical temperature, many physical properties are modeled using a power law

$$\langle M(T) \rangle \sim (T - T_C)^{1/8}$$

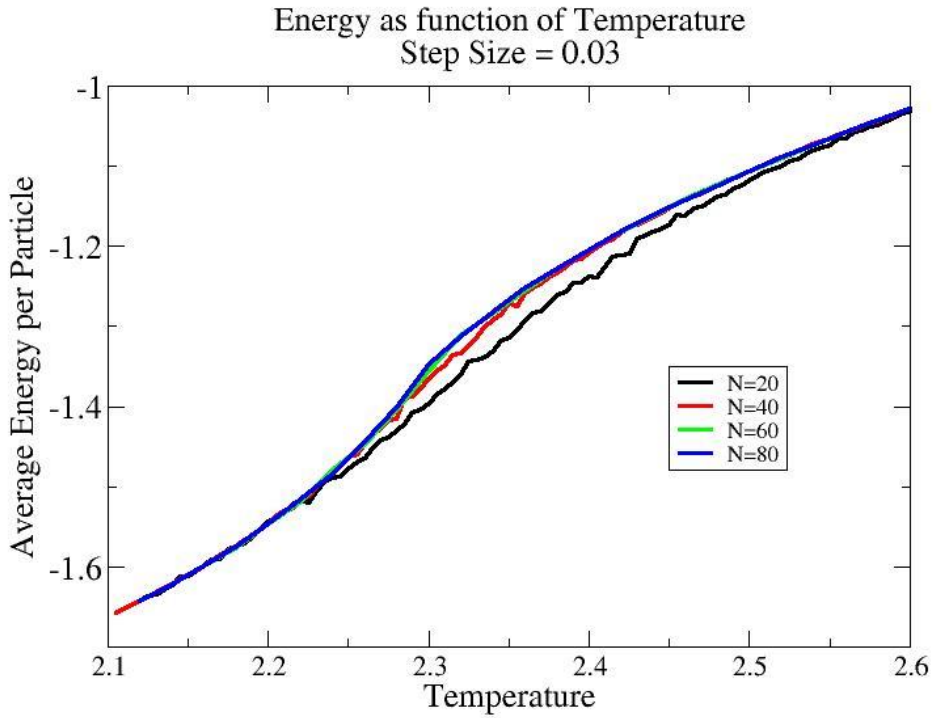
$$C_V(T) \sim |T_C - T|^0$$

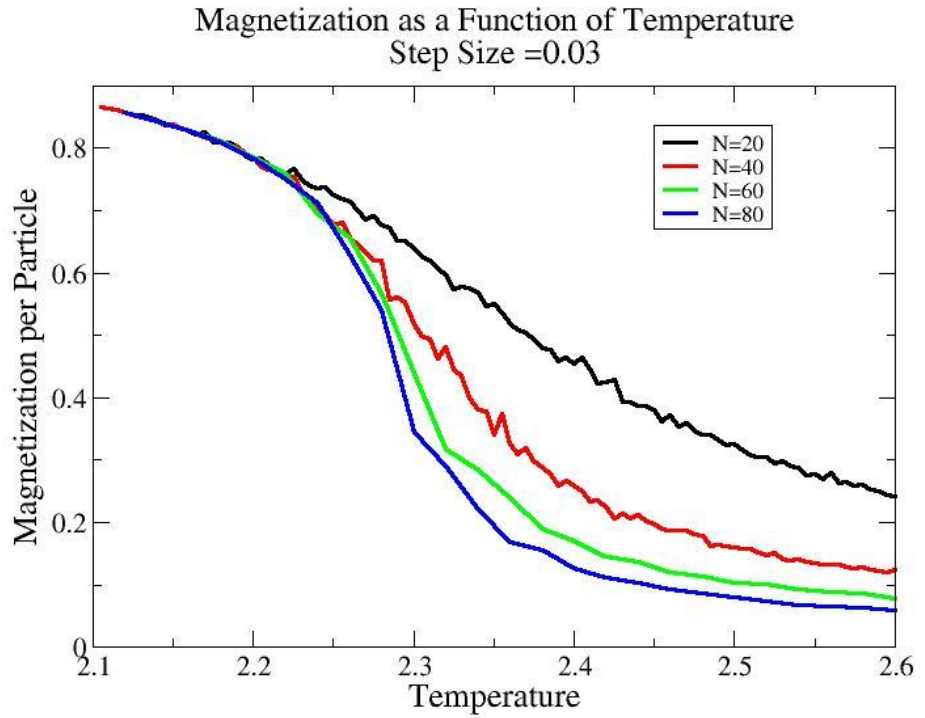
$$\chi(T) \sim |T_C - T|^{7/4}$$

- We can also model a correlation length by $\xi(T) \sim |T_C - T|^{-1}$ which is on the order of lattice spacing above the Curie Temperature
- We can relate the behavior of finite lattices to the infinite lattice using

$$T_C(L) - T_C(L = \infty) = aL^{-1}$$

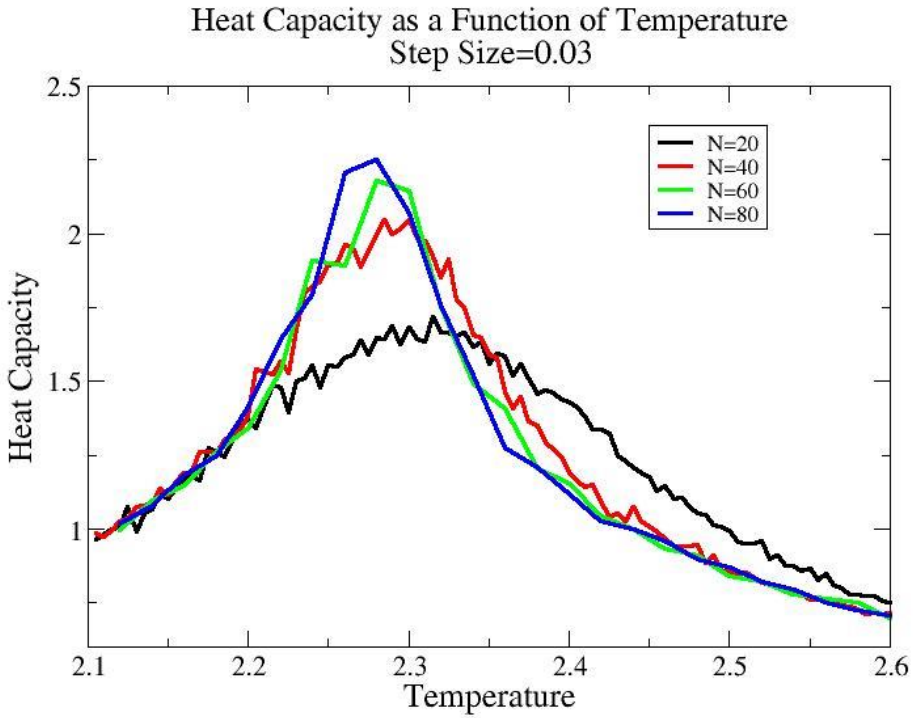
Results – Study of Phase Transition

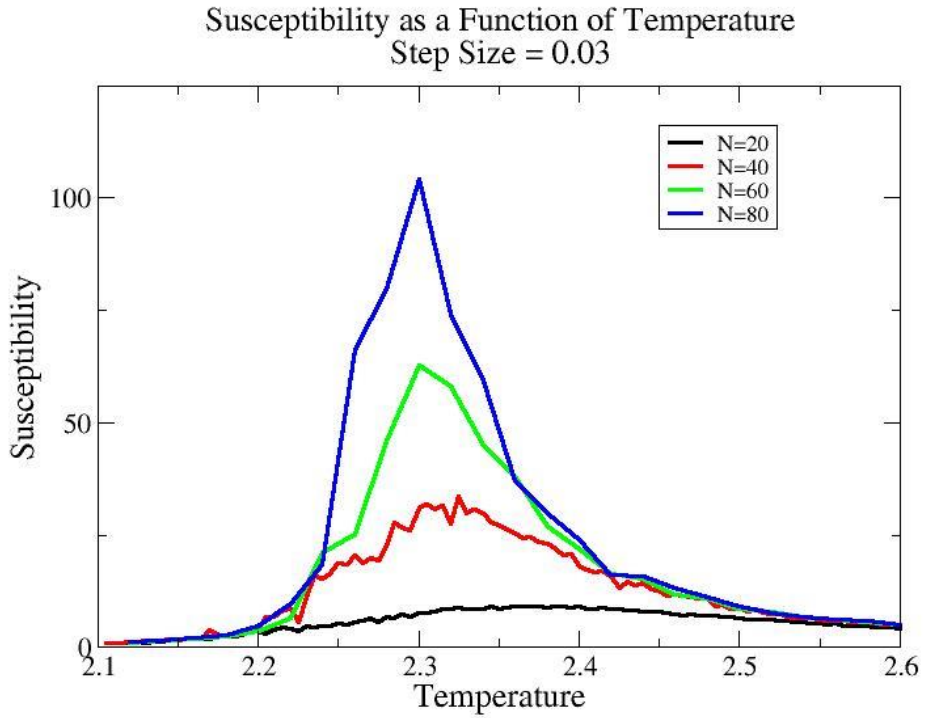




- 100,000 cycles at step size of 0.03

Results – Study of Phase Transition





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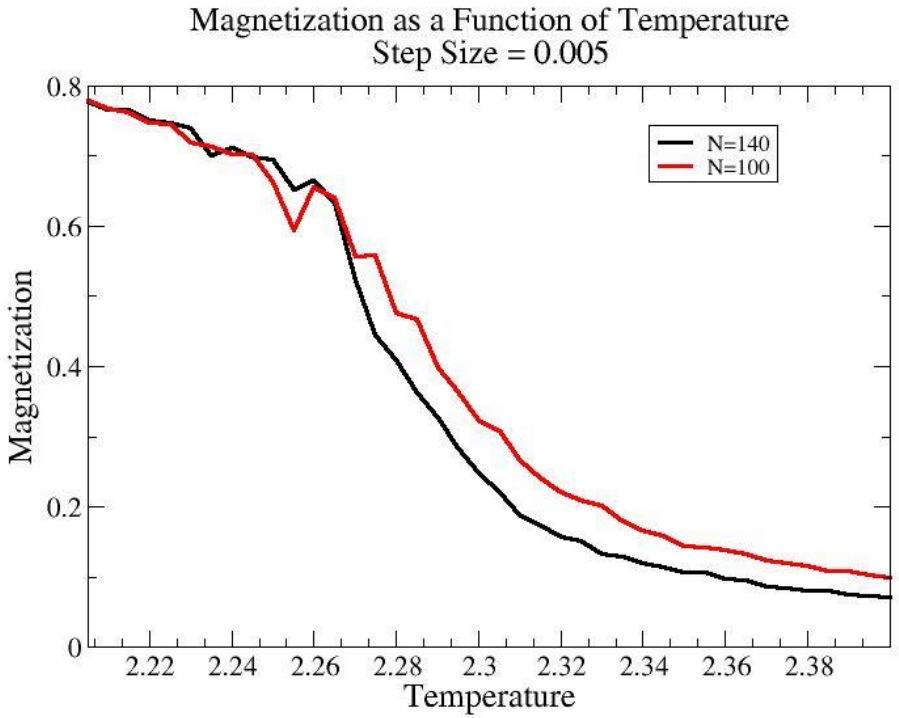

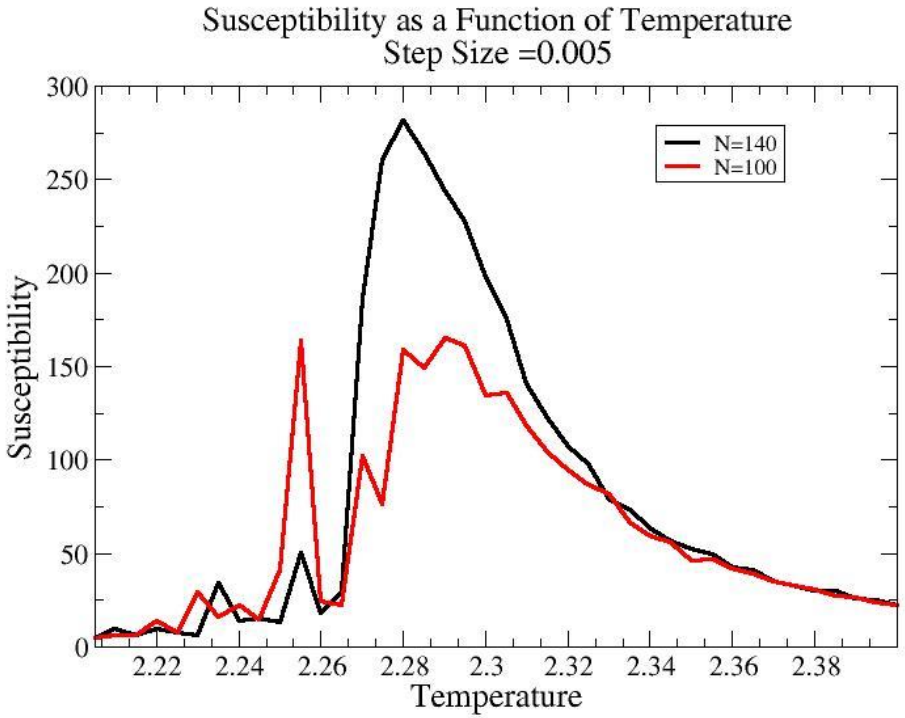

- 1,000,000 cycles at step size of 0.005

Results – Study of Phase Transition

- We can use the relation $T_C(L) - T_C(L = \infty) = aL^{-1}$ we get

L	T_C	ϵ
20	2.195	0.033
40	2.233	0.016
60	2.237	0.014
80	2.242	0.012
100	2.262	0.0031
140	2.264	0.0022

- We see that as L gets larger, the curie temperature approaches the value in an infinite lattice.

Conclusions

- I created a Monte Carlo Simulation which employed the Metropolis Algorithm to solve the 2D Ising Model and study magnetic phase transitions on a lattice
- This code was verified using analytic results for the simple 2 by 2 lattice
- I explored the energy probability distribution at different temperatures and connected this quantity to the heat capacity.
- I saw evidence of a 2^{nd} order phase transition in the magnetic material
- I used finite size scaling relations to relate the Curie temperature on a finite lattice to the critical temperature for an infinite lattice