2D and 3D Ising model implementation and Ayalysis

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We will simulate the 2d ising model and 3d ising model. From the result, we observe that the critical temperature is 2.3K. blabla, Chen will finish it later.

I. Overview

1. Introduction of Ising model

1.1. Ising Model

Isingmodel is a mathematical model to describe the ferromagnetismproperty of materials. It is first invented by the physicist Wilhelm Lenz, and is then gave to his student ErnstIsing, after whom the model is named,as a problem.

1.2. Ferromagnetism

Ferromagnetism is a basic mechanism of certainmaterials(such as iron), thatforms permanent magnetsor attracted to magnets. Ferromagnetism can be divided into severaldistinguishedtypes, such as ferrimagnetism, which is the strongest one, and some types response weakly, such asparamagnetism, diamagnetism andantiferromagnetism. Ferromagnetismdescribesthe chemical make-up,crystalline structure and also microstructure of materials, and it is arises due to two effects from quantum mechanics: spin and the Pauli Exclusion Principle. Generally speaking, the ferromagnetism of materials come from the spin property of electrons.Electronshas a quantum mechanical spin, which arises the magnetic dipole moment of it. The spin of the electron can only be in two states, either withmagneticfield pointing "up" or "down", and it is the mainly source of ferromagnetism. When these magnetic dipoles pointing in the same direction, then the tiny magnetic fields add together to a much larger macroscopic field. And for materials made of atoms with filled electron shells, the magnetic momentof every electron is cancelled by the opposite moment of the second electron in the pair, such result in a total dipolemomentof zero. So, only atoms with unpaired spins can have a net magnetic moment. So only materials with partially filled shells have ferromagnetism.

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II. 2D Ising model

1. Basic Idea

Consider a d-dimensional lattice, each lattice site $k \in \Lambda$ is a discrete variable which indicate the spin state of the site. There is aninteractionJ_{ij} between anytwo adjacent sites $i, j \in \Lambda$, and for each site $j \in \Lambda$, there is an external magnetic field h_j interacting with it. The energy is approximated using the Hamiltonian equation:

$$\mathcal{H}(\sigma) = -\sum_{\langle i,j \rangle} J_{ij}\sigma_i\sigma_j - \mu \sum_j h_j \sigma_j \tag{1}$$

Here we ignore the external magnetic term, so the Hamiltonian equation becomes

$$\mathcal{H}(\sigma) = -\sum_{\langle i,j \rangle} J_{ij}\sigma_i\sigma_j \tag{2}$$

2. 2D Model overview

2.1. Hamiltonian

Consider the lattice Λ, denote the lattice site σ_{ij} to be the site in location (i, j), and the Hamiltonian is

$$\mathcal{H}(\sigma) = -\sum_{\langle (i,j),(i',j') \rangle} J_{(i,j),(i'j')}\sigma_{ij}\sigma_{i'j'} \tag{3}$$

Updating for flipping the spin in site (i, j) will involve sites around it, which are $(i-1, i)$, $(i+1, j)$, $(i, j-1)$, $(i, j+1)$. So when updating one single site $\sigma_{i,j}^{new} = -\sigma_{i,j}$, the change in Hamiltonian will be

$$\Delta\mathcal{H} = 2(\sigma_{i-1,j} + \sigma_{i+1,j} + \sigma_{i,j+1} + \sigma i, j-1)\sigma_{i,j} \tag{4}$$

2.2. Updating Algorithm - One Sweep

1. For each site in the lattice, calculate the $\Delta\mathcal{H}$ according to flipping the spin of this site.
2. If $\Delta\mathcal{H} < 0$, accept the flip, update the spin state.
3. If $\Delta\mathcal{H} > 0$, flip the spin state of site (i, j) with probability $\exp(\delta\mathcal{H}/kT)$. Which is to generate a random number between $[0, 1]$. If the random number

if less than the probability, then accept the update, if not, reject the update.

Note: Using periodic boundary conditions.

2.3. Updating Algorithm - Monte Carlo Process

1. Perform N_{therm} sweeps for warm up, to reach a relatively stable status
2. Perform N_{meas} sweeps for measurement, take each 100 record as a measurement.
3. Output the data and perform the calculation (some expectation values).

2.4. Critical Temperature

For 2DIsingmodel, there is a critical temperature, at which the material will have a transition in phase. We are using two approaches to obtain the critical temperature here:

1. Energy - Temperature figure
   Observe theexpectation value of energy according to thetemperature, andthe critical temperature should locate in where the curve has thegreatestslope. In which

$$\langle E\rangle = \frac{1}{2}\langle\sum_{i}^{N}\mathcal{H}_i\rangle = \frac{1}{2}\langle -J\sum_{i}^{N}\sum_{j_{nn}} s_i s_j\rangle$$

2. Heat Capacity - Temperature plot
   Observe the heat capacity according to the temperature, and thecriticaltemperature should locate in where the heat capacity has the greatest value. In which

$$C = \frac{\partial E}{\partial T} = \frac{\Delta E^2}{k_b T} = \frac{\langle E^2\rangle - \langle E\rangle^2}{k_b T^2}$$

3. Analytic solution

3.1. Partition Function

Now discuss the Analytic solution of the Ising model in a square lattice Λ with N sites, and using periodic boundary condition, which is exactly what we are using in our experiment.
Denote J_h and J_v to be number of horizontal and vertical coupling respectively. And denote

$$K = \beta J_h \qquad L = \beta J_v$$

In which, $\beta = 1/(kT)$, and T is the absolute temperature and k is the Boltzmann's constant. Thus the partition function can be written as

$$Z_N(K,L) = \sum_{\{\sigma\}}\exp\left(K\sum_{\langle i,j\rangle_H}\sigma_i\sigma_j + L\sum_{\langle i,j\rangle_V}\sigma_i\sigma_j\right) \quad (5)$$

3.2. Critical Temperature

The analytical critical temperature T_c is obtained using the Kramers-Wannier duality relation, which in this case gives

$$\beta F(K^*, L^*) = \beta F(K,L) + \frac{1}{2}\log[\sinh(2K)\sinh(2L)]$$

In which, $F(K,L)$ is the free energy per site, and also have the following relations

$$\sinh(2K^*)\sinh(2L) = 1$$
$$\sinh(2L^*)\sinh(2K) = 1$$

And because there is only one critical temperature, so that use the assumption that there is only one critical line in the (K,L) plane, the duality relation above implies that

$$\sinh(2K)\sinh(2L) = 1$$

And for our square lattice, $J_h = J_v$, which is the isotropic case, the relation for critical temperature T_c is

$$\frac{kT_c}{J_h} = \frac{2}{\ln(1+\sqrt{2})} \approx 2.26918531421$$

4. Numerical result

—————————- TODO —————————-

III. 3D Ising model

In previous section, we introduced the general idea of 2D Ising model, which is based on a 2D plane. In this section, we are going to talked about 3D ising model, which as the name suggested, is based on 3D space. We will perform our experiment in a square cube lattice, which contain N sites. Ising model is originally designed to describe the magnetism of materials, so we'll also assuming our system is a magnetization system, and examine some related physical.

1. 3D Model overview

1.1. Hamiltonian

In 3D case, the Hamiltonian can be written as

$$\begin{aligned}\mathcal{H} = -J \sum_{i,j,k=1}^{N} (&S_{i-1,j}S_{i,j} + S_{i,j}S_{i+1,j} \\ &+ S_{i,j-1}S_{i,j} + S_{i,j}S_{i,j+1} + S_{i-1,k}S_{i,k} \\ &+ S_{i,k}S_{i+1,k} + S_{i,k-1}S_{i,k} + S_{i,k}S_{i,k+1} \\ &+ S_{j-1,k}S_{j,k} + S_{j,k}S_{j+1,k} + S_{j,k}S_{j,k-1} \\ &+ S_{j,k}S_{j,k+1}) - \mathbf{H}\sum_{i}^{N} \mathbf{s_i}\end{aligned} \tag{6}$$

Where $\mathbf{H}$ is the external force, for simplicity, we ignore the external force in our experiment. So that $\mathbf{H} = 0$.

1.2. Magnetic Property

The magnetization is denoted as M, which of a given configuration can be given by

$$M = \frac{1}{N}\sum_{i}^{N} S_i \tag{7}$$

The magnetic susceptibility is denoted as χ, and is calculated as

$$\chi = \frac{1}{kT}(\langle M^2\rangle - \langle M\rangle^2) \tag{8}$$

In which, k is Boltzmann's constant, and T is the temperature of the system.

2. Numerical result

——————————— TODO ———————————

IV. parallel(cuda, matlab)

1. CUDA

Numerical approach of Ising model requires computation on each lattice site, which when lattice becomes really large scaled will become very computationally heavily. And because the calculation for each site only require values from adjacent sites, so we want to compute the lattice parellelly. So we decide using cuda to speed up the computation process.
The basic idea of using cuda to implement Ising model is first to divide the sites into two parts, one part of even index, and another with odd index. Each sites is assigned into a cuda thread. Then in each iteration, update the even sites, using the updated values to update the odd sites, then synchronize the data in each thread to global variable. The 2d Ising scheme is demonstrated in following figure.

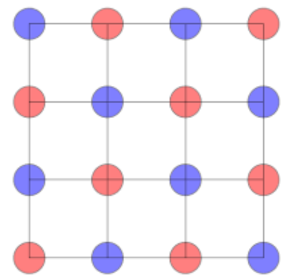

FIG. 1. 2D Ising Model Cuda Scheme

Using the scheme above, apply metropolis algorithm to Ising model, we obtained following numerical results.

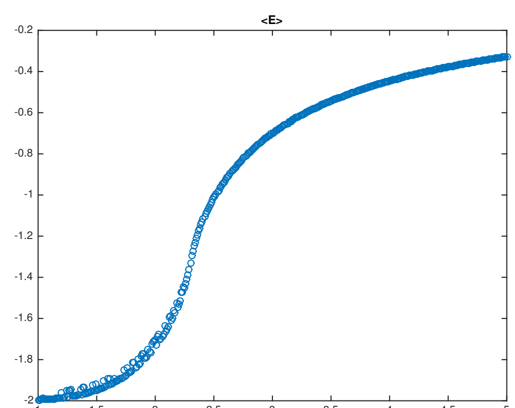

FIG. 2. Expectation value of energy, with lattice size 256×256, take 1000 warmup steps, and 1000 measurement steps, measure for temperature ranging from 1.0 to 5.0

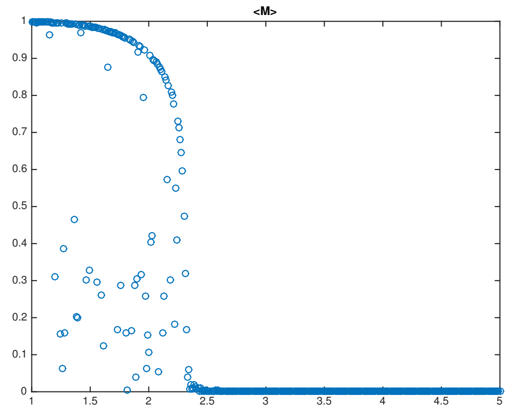

FIG. 3. Expectation value of magnetization, with lattice size 256×256, take 1000 warmup steps, and 1000 measurement steps, measure for temperature ranging from 1.0 to 5.0

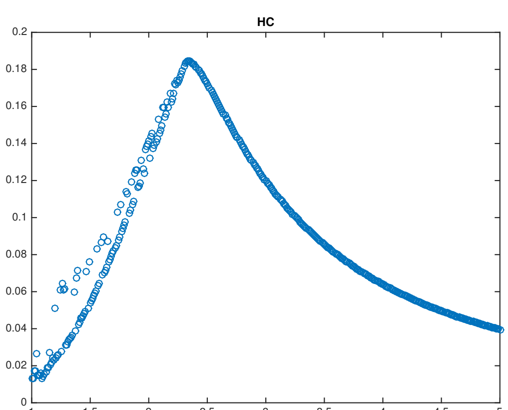

FIG. 4. Expectation value of heat capacity, with lattice size 256×256, take 1000 warmup steps, and 1000 measurement steps, measure for temperature ranging from 1.0 to 5.0

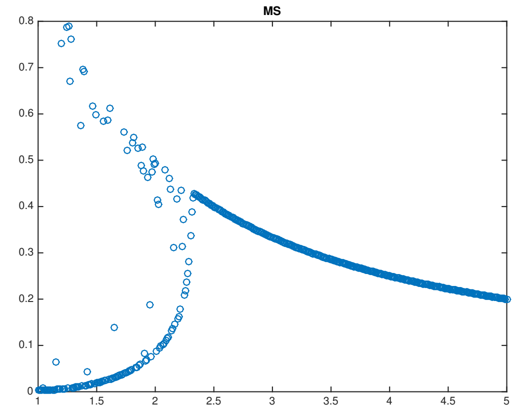

FIG. 5. Expectation value of magnetization susceptibility, with lattice size 256×256, take 1000 warmup steps, and 1000 measurement steps, measure for temperature ranging from 1.0 to 5.0

From the figures above, it can be observed that the critical temperature is about 2.2, which is close to the analytic solution.

2. Matlab

—————————- TODO —————————- In this project, expect using c programs for computing and parellization, we also use Matlab to animate the Ising model convergence process. To speed up in Matlab, we use parfor to execute loops in parallel.

V. Conclusion

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VI. APPENDICES

1. Description of code

In this project, we use C codes and Matlab codes, the description and usage of each code is listed below.

1.1. C Code

To compile the code, please use the `Makefile` we provided, and state each flag as you need:

`make ising`**:** Compile 2d ising model simulation code

`make cuda`: Compile 2d ising model simulation code using cude. To compile with cuda, you have to make sure that your environment supports cuda libraries.

To run the code, you can run single simulation by typing input parameters, or using the bash script we provide.

`./src/ising.o T SIZE`: Run single case for 2D Ising model with C, where `T` is the temperature, and `SIZE` is the lattice size

`./src/ising2d.o T WARM MEAS WARP`: Run a single case for 2D Ising model with cuda, where `T` is the temperature used for this simulation case, `WARM` is number of warmup steps, `MEAS` is the number of measurement steps, and `WARP` is the warp steps, which is take a record among WARP steps when measuring.