**Ising model**

**1. Introduction**

**1.1 Ising model**

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

**1.2 Ferromagnetism**

Ferromagnetism is a basic mechanism of certain materials (such as iron), that forms permanent magnets or attracted to magnets. Ferromagnetism can be divided into several distinguished types, such as ferrimagnetism, which is the strongest one, and some types response weakly, such as paramagnetism, diamagnetism and antiferromagnetism.

Ferromagnetism describes the 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. Electrons has a quantum mechanical spin, which arises the magnetic dipole moment of it. The spin of the electron can only be in two states, either with magnetic field 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 moment of every electron is cancelled by the opposite moment of the second electron in the pair, such result in a total dipole moment of zero. So, only atoms with unpaired spins can have a net magnetic moment. So only materials with partially filled shells have ferromagnetism.

**2. Model Implementation in 2D**

**2.1 Basic Idea**

Consider a d-dimensional lattice, each lattice site  is a discrete variable  which indicate the spin state of the site. There is an interaction  between any two adjacent sites, and for each site, there is an external magnetic field  interacting with it. The energy is calculates as

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**2.2 2D Model Algorithm**

**2.2.1 Hamiltonian - Energy**

Consider the lattice, denote the lattice site  the site in location, and the Hamilton is calculated as



Updating for flipping the spin in site  will involve sites around it, which are, , , . So when updating one single site,  the change in Hamiltonian will be

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**2.2.2 Updating Algorithm**

**2.2.2.1 One sweep**

Step 1: For each site in the lattice, calculate the  according to flipping the spin of this site.

Step 2: If, accept the flip, update the spin state.

Step 3: If, flip the spin state of site  with probability . Which is to generate a random number between. If the random number if less than the probability, then accept the update, if not, reject the update.

Note: For boundary sites, using sites on other boundaries with the same index to update it.

**2.2.2.2 Monte Carlo Process**

Step 1: Perform  sweeps for warm up, to reach a relatively stable status

Step 2: Perform  sweeps for measurement, take each 100 record as a measurement.

Step 3: Output the data and perform the calculation (some expectation values).

**2.3 Critical Temperature**

For 2D Ising model, there is a critical temperature, at which the material will have a transition in phase. To obtain the critical temperature, there are two approaches:

1. Energy – Temperature plot

Observe the expectation value of energy according to the temperature, and the critical temperature should locate in where the curve has the greatest slope. In which



2. Heat Capacity – Temperature plot

Observe the heat capacity according to the temperature, and the critical temperature should locate in where the heat capacity has the greatest value. In which

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**3. CUDA Implementation in Ising Model**