Ising Model Design Document

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1 Introduction

This simulation is an implementation of the Ising model. This is a model for ferromagnetic material. This code will investigate the phase transition and hysteresis of the Ising model.

2 Mathematical Model

The system consists of spins on a square lattice. Each spin σ is points either up or down, represented as a $+1$ or -1.

The Hamiltonian for this system is:

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j - H \sum_i \sigma_i$$

where $\sum_{\langle ij \rangle}$ denotes a sum over i and its nearest neighbors (up, down, left, right) j. The interaction between neighboring spins is set by the interaction strength J. We can also apply an external magnetic field H.

3 Computational Model

To simulate this system we will sample states at a temperature T. To generate these states we'll use the Metropolis Hasting algorithm we discussed in class. The procedure for a single Monte Carlo (MC) step is as follows

1. Chose a random spin i.
2. Calculate the energy $E_{inital} = \mathcal{H}$
3. Flip the spin $\sigma_i = -\sigma_i$
4. Calculate the new energy $E_{final} = \mathcal{H}$

5. If the energy is now less $E_{inital} < E_{final}$ accept the change.

6. If the energy is greater accept it with a probability $exp(-\frac{\Delta E}{k_b T})$.

7. Otherwise flip the spin back

8. Repeat this process a number of time equal to the number of spins in the system. Hint: you only need to calculate the change in energy for flipping a single spin. This should not involve the entire system. Only nearest neighbors.

4 Initial Conditions

The system will be initialized with random initial conditions. Each spin has a 50% chanse of being in the up $+1$, or down -1 state.

5 Boundary Conditions

We will employ periodic boundary conditions. Spins at the right wall will have spins at the left wall as their neighbors and vice versa.

6 Observables

We will study the magnetization and the order parameter of the system. The magnetism is $m = \frac{\sum_i \sigma_i}{N}$ where N is the total number of spins. Closely related is the order parameter $\phi = |m|$ that tells us how aligned the spins are.

7 Experiments

This code will run two experiments

1. Calculate ϕ as a function of T from on T $=[10, 0]$. Taking 100 MC steps at each point to equilibrate, then averaging over 100 MC steps for the measurement.

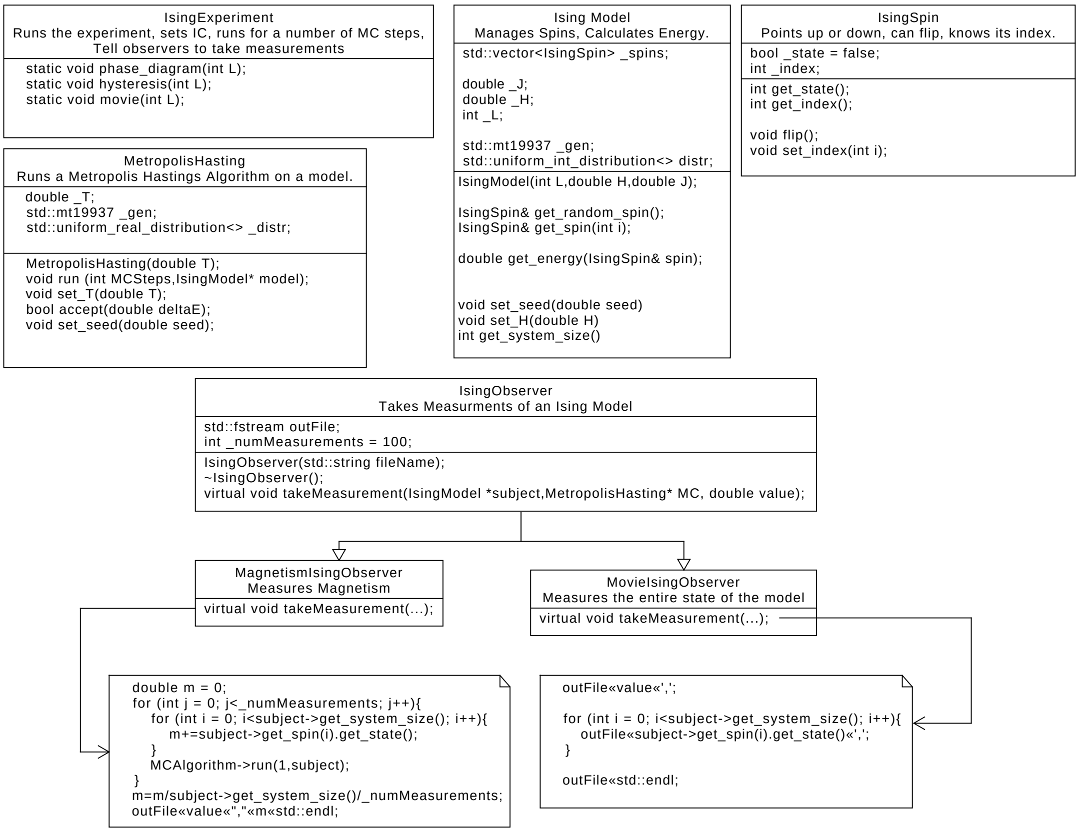
2. Calculate m as a function of H for $T = 5$ and $T = 1$. Take H from 10 to -10 and back again for the same system. Taking 100 MC steps at each point to equilibrate, then averaging over 100 MC steps for the measurement.

8 Simulation Interface

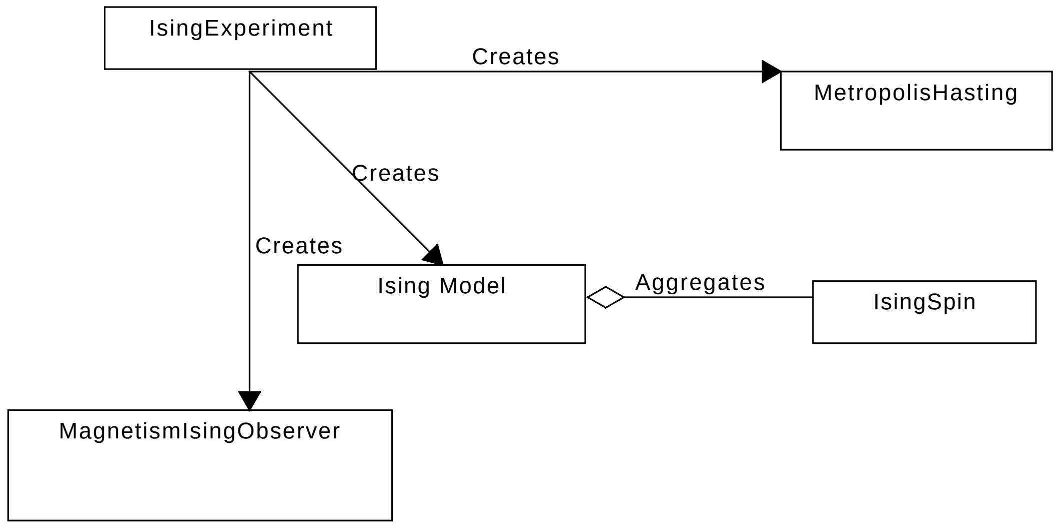
This simulation will take in a command line argument for system size. It only accepts positive integers.

9 Code Structure

Class Diagram



Object Diagram



Runtime Diagram