Computational Physics 2024 Project 3: The Ising Model

The Ising model is a simple model for the emergence of ferromagnetism in some metals. It is defined as follows: suppose a sequence of spins $\sigma_i \in \{-1, 1\}$ live on a lattice of N sites. One can define an adjacency matrix S_{ij} where $S_{ij} = 1$ if the spins are neighbors and 0 otherwise. This allows one to write an arbitrary lattice in an arbitrary number of dimensions. The Hamiltonian is then given by

$$H = -J \sum_i S_{ij} \sigma_i \sigma_j$$

where J is the exchange parameter. At finite temperature, the spins randomly flip up and down due to thermal excitations, and for some lattices with $J > 0$ the model exhibits a transition as a function of temperature: the average magnetization $M = \frac{1}{N} \sum_i \sigma_i$ is zero (the paramagnetic state) above $T > T_c$. while below it M is nonzero (corresponding to the ferromagnetic state).

Begin by:—

1. Identifying **as many** algorithms as you can for simulation of the Ising model. The Metropolis algorithm described in class is the simplest, but there are others *[the Wolff algorithm is another]*. Make a table explaining the benefits and use cases for each one. Use internet resources—and be thorough! Imagine you're trying to convince your research advisor of why you're choosing one approach over another.

2. Implementing **one or more** of them.

3. Studying the magnetization as a function of simulation time at a selection of temperatures. How many iterations are needed to equilibriate the system?

4. Using these to determine the phase transition temperature in 1, 2 and (optionally) 3 dimensions for a square lattice.

5. Estimate the number of random numbers used in your study. How does this compare to the period of the Mersenne twister random number generator? What about the rand() function in the standard C library?

Ideas for further exploration (choose one)

1. Plot the magnetization as a function of temperature and determine the critical exponents. (fit the magnetization to a power law near the transition).

2. What happens on a triangular lattice? What about a lattice on a sphere (I can give you one if you like!). You could explore a variety of different lattice topologies.

3. Role of disorder: Suppose the exchange interactions between adjacent sites are not the same but random numbers normally distributed about some mean value of J? How does the transition look as a function of the width of this distribution?

4. Rather than flipping the sites, you can exchange adjacent sites. This conserves the overall magnetization of the system, and hence the result is called the conserved Ising model. The exchanges are called Kawasaki exchanges. It's a good model of liquid-liquid phase separation, interestingly—can you see why?

5. What happens if the allowed spins are different from just allowing two values? If you allow N different spin states per lattice site, you get something called a Potts model. If you allow spin to be a continuous (but 2D) parameter, you get something called the X-Y model. The transitions for these models are very different. Feel free to talk to the instructor for advice on exploring these.