Monte Carlo simulation of two-dimensional Ising model

The two-dimensional square-lattice Ising model is one of the simplest statistical models to show a phase transition. The model consists of discrete variables that represent magnetic dipole moments of atomic "spins" that can be either +1 or −1. The spins are arranged in a graph, usually, a lattice, and each spin interacts with its neighbors. Neighboring spins that align have lower energy. The system has the lowest energy when all spins are aligned but thermal fluctuations disturb the system, thus creating the possibility of different structural phases. The model allows the identification of phase transitions as a simplified model of reality.

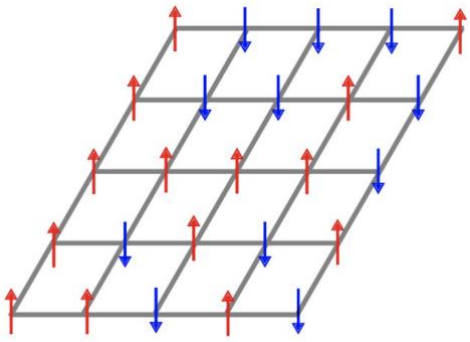
The energy of the system (with the assumptions that the spins are identical) is written as

$$E = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j - h \sum_i \sigma_i \qquad (1)$$

Where J is spin-spin interaction and assumed to be positive. $\langle ij \rangle$ means that the sum run only between *j*'s that are neighbors of *i*. h is an external magnetic field.

It has been shown that no phase transition to a ferromagnetic ordered state occurs in one dimension at any temperature. Can you explain why without using math? However, the same argument is not true for two and higher dimensions. Why is this so significant?

The simulation program:



The task is to create a simulation code for Ising model on a 2D square lattice with periodic boundary conditions and explore how to make an efficient OpenMP parallelization. Consider a square lattice of N^2 nodes that each node contains one spin. The system is period, meaning that spins at the edges interact with spins on opposing edge. To evolve the system, you must use Monte Carlo simulations with Metropolis criterion. In each step, you flip a random spin, calculate the energy change, and accept or reject the move with a probability of

$$\begin{cases} \exp(-\beta \Delta E) \geq P & \text{accept} \\ \exp(-\beta \Delta E) < P & \text{reject} \end{cases}$$

where $\Delta E = E_{new} - E_{old}$ and $\beta = 1/k_B T$. You can speed up the system evolution by using other moves but make sure detailed balance is satisfied. $P \in [0:1[$ is a uniform random number.

Note: you do not need to calculate the full summation in equation 1 to obtain ΔE.

1) Perform simulations for multiple temperatures (reduced temperature: $t = k_B T/J$) and try systems of different sizes that are large enough significant work to be performed in parallel. E.g. $N = 500, 1000, 2000$. You can choose to set $h = 0$ or something of order J for all simulations.
2) Plot total energy per spin as a function of reduced temperature.
3) Plot magnetization as a function of reduced temperature.
4) Obtain the critical temperature in the system (as a function of system size).
5) Obtain the heat capacity for different reduced temperature.

   Hint: use $C_V \propto \frac{\langle E^2 \rangle - \langle E \rangle^2}{\text{Number of spins}}$

In the project you need to parallelize the spin flipping such that it gives reproduceable results when running on a different number of threads. Part of the project is to decide what reproduceable means in this context, and what the consequence of flipping spins in parallel is for the result. You may need to change both the strategy for the parallel and the serial algorithm to get reproduceable results.

Variants of the proposed project:

- Model: you may implement a similar physical model such as the Heisenberg model
- Parallelization: you may choose a different parallelization hardware and strategy:
    - GPUs: probably requires CUDA to get decent performance and atomic access to cells in the domain boundaries.
    - Distributed cluster: use MPI and communicate boundary values in each iteration.