1. **Building a Monte Carlo simulation of the two-dimensional Ising model.** This assignment centers on Monte Carlo simulations of a two-dimensional Ising magnet. The first part of the assignment is to develop a Metropolis Monte Carlo code to simulate an Ising magnet at temperature T. You will be performing simulations on a 20×20 lattice of spins with periodic boundary conditions. You can either write such a simulation from scratch in a language of your choosing, or work through the Mathematica notebook (ps9.nb) to finish developing the program that I started for you. You do not need to submit any work for this problem, but you will need your working code to be able to work on the next problem. (And I don't want you downloading some completed code off the internet.)

   If you choose to do the Mathematica option, read through ps9.nb line by line. You will find the following three things to fix/fill in, after which you should have a functioning simulation code.

   (i) I wrote a function called Neighbors, which, given a lattice site, determines which other lattice sites are the nearest neighbors. I did not adequately implement the periodic boundary conditions. Fix this.

   (ii) The energy function for the Ising magnet in the absence of an external field ($h = 0$) can be written as

   $$E = -J{\sum_{i,j}}' s_i s_j,$$

   where we will set $J = 1$, the sum is taken over distinct pairs of nearest neighbors i and j, and $s_i = \pm 1$ is the state of the spin at site i. Notice that the sum could be split into two parts:

   $$E = -\frac{J}{2} \sum_i \left(s_i \sum_{j \in n(i)} s_j \right), \tag{1}$$

   where $j \in n(i)$ indicates that j is taken from the set of i's neighbors. The factor of $1/2$ prevents double counting. Without it you would be counting the interaction between spins 1 and 2 twice, first as the $s_1 s_2$ term and then as the $s_2 s_1$ term. Since these two terms are identical, we include them both and correct by the factor of $1/2$. Let us call the parenthetical term in Eq. (1) the "single spin energy" for site i. The total energy is found by combining these single spin energies for each spin in the lattice. Where prompted in the Mathematica file, write a function to compute the single spin energy.

   (iii) I implemented the Monte Carlo procedure in ps9.nb using a function I called SlowMCStep, which computes the energy of the entire Ising magnet before and after a proposed spin flip. This implementation is wasteful. Since most of the magnet is not altered by the spin flip, most of the energy calculation will not be affected by the flip. Write a FastMCStep function which instead uses the SingleSpinEnergy function to evaluate whether or not to accept a Monte Carlo move. Your FastMCStep function should be much faster than the slow version.

2. **Using your Ising simulation.** (i) In the absence of an external magnetic field (i.e., $h = 0$), the transition to a ferromagnetic state upon decreasing temperature is second order. In other words, the magnetization per spin $m = N^{-1} \left\langle \sum_{i=1}^{N} s_i \right\rangle$ changes continuously but not smoothly at $T = T_c$. Try to confirm this fact by computing $m(T)$ from several Monte Carlo trajectories above and below T_c. Estimate the sampling error associated with each computed value of m, and describe the procedure

you use to do so. Provide a plot of m as a function of T (showing error bars), along with snapshots of the system at a temperature below T_{c}, a temperature very close to T_{c}, and a temperature above T_{c}.

(ii) Your results will differ from the exact behavior of this system (determined mathematically by Lars Onsager) in several respects. For example, the apparent transition in your simulated system should not occur precisely at $k_{\mathrm{B}}T_{\mathrm{c}} = 2.269J$. (Note that, in the code, the unit of temperature is J/k_{B}.) The transition should also appear smooth (rather than exhibiting a sharp kink). Explain both of these deviations.

(iii) Singularities at the critical point arise from correlated fluctuations of spins separated by macroscopically large distances. Try to confirm the existence of long-ranged correlations at the critical point by computing $c(r_{ij}) = \langle s_i s_j \rangle - \langle s_i \rangle \langle s_j \rangle$ as a function of $r_{ij} = |\mathbf{r}_i - \mathbf{r_j}|$ (the distance between spins i and j) at several temperatures above and below the critical point. Plot your results.