Exercise 2: Metropolis Algorithm for the Ising Model

In this second exercise we will study the thermal phase transition that occurs in the two-dimensional Ising model, the first example of a dynamic system. The Ising model is defined by the Hamiltonian

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j, \tag{1}$$

where the spins $\sigma_i = \pm 1$ correspond to "up" and "down" spins and the sum runs over all pairs of nearest neighbor spins. We will consider the ferromagnetic case with $J > 0$.

For the underlying lattice we will consider a square lattice of linear extent L and $N = L \times L$ sites. In order to minimize finite-size effects we will use *periodic* boundary conditions, which results in a lattice with a total of $2N$ bonds.

To identify and characterize the thermal phase transition we will investigate thermal averages for a number of observables, which are generally defined as

$$A(T) = \frac{1}{Z} \sum_i A_i \exp(-\beta E_i)\,,$$

where Z is the partition function of the system, the sum runs over all possible spin configurations i, A_i and E_i are the values which the observable A and energy E have for a given configuration i, and β is the inverse temperature $\beta = 1/(k_B T)$.

We will calculate these thermal averages via Monte Carlo sampling for a range of temperatures $T = 0.1, 0.2, \ldots, 4$ (where we fix units by setting $J = 1$) and system sizes $L = 8, 16, 32$.

1. Implement a **single spin-flip Metropolis algorithm** for this 2D Ising model. (You can build on your code for the percolation problem.)

2. Plot Monte Carlo averages of the **magnetization** $M = \sum_i \sigma_i$ for the full temperature range. Perform measurements only after an initial set of – say – 10,000 thermalization sweeps where one sweep corresponds to N attempted spin flips. After this thermalization phase, perform one measurement for every sweep.

3. Plot Monte Carlo averages for the **Binder cumulant** of the magnetization $U = 1 - \frac{\langle M^4 \rangle}{3\langle M^2 \rangle^2}$ for the full temperature range.

4. Plot Monte Carlo averages for the **energy** E for the full temperature range.

5. Plot Monte Carlo averages for the **specific heat** C_v, which you can estimate either by (numerically) calculating the derivative dE/dT of the energy curve above, or more directly via $\langle C_v \rangle = \beta^2/N(\langle E^2 \rangle - \langle E \rangle^2)$ by measuring Monte Carlo estimates for E^2.

6. From the two results plotted above can you reproduce the estimate of the thermal phase transition $T_c = 2/\ln(1+\sqrt{2}) \approx 2.269186$ for the square lattice?

7. Implement a **cluster update**, such as the Wolf algorithm explained in the lecture.

8. *Optional exercise:* For a fixed system size $L = 32$ perform $2^{16} = 65536$ measurements of the energy at the thermal transition temperature $T = 2.269186$ for the single spin-flip algorithm and the cluster update algorithm.
   For both sequences perform a **binning analysis** of the sampled energies – for which algorithm does the error converge?