Lecture 12: Exercise on the Multiple Histogram Method (MHM)

Choose a model with a phase transition. The standard choice is the grafted polymer model of Lesson 6. Otherwise, you should describe the model in the submitted notes. Temperature T, or better, its inverse β (with $k_B = 1$), is a parameter whose variation leads to a change in the phase of the system.

Implement the MHM to compute the energy variance per degree of freedom, $C(\beta) = \frac{1}{N}(\langle E^2 \rangle - \langle E \rangle^2)$ (proportional to the specific heat, $C^{\text{sp}} = \beta^2 C = N^{-1}\partial_T \langle E \rangle$). The following procedure assumes that the model follows a finite-size scaling close to the critical point at β_c,

$$C(\beta) = N^{2\phi-1} f\left((\beta - \beta_c)N^{\phi}\right) \tag{2}$$

The scaling function f, in this case, has a maximum, i.e. a "peak".

For different system sizes N, compute $C_N(\beta)$ for a fine mesh of $\beta \in [0, \beta_{\max}]$ covering the finite-size proxy of the phase transition of the model, which is the peak of $C_N(\beta)$. Find peaks' position β_N and plot them as a function of $N^{-\phi}$ with crossover exponent ϕ to be determined by trying to align points in the $y = \beta_N$ vs $x = N^{-\phi}$ diagram. For the grafted polymers, a $\phi = 1/2$ should work fine.

Try to extrapolate the infinite-size limit β_c from the trend of β_N vs N^{ϕ} points. It is the intercept with the y-axis of a line going through the points. This method has a single parameter ϕ. Including finite-size corrections amounts to fit points $y = \beta_N$ with $y(x(N)) = N^{-\phi}(1 + AN^{-\Delta}) = x(1 + Ax^{\phi\Delta})$ including a second parameter A.