

EXERCISES  
**Computational Materials Science**

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SHEET 2

Exercise 2: Monte Carlo simulations for the Ising model

a) Write a program to simulate the Ising model with nearest neighbor interaction on a 2d square lattice by means of Monte Carlo simulations. And with the heat bath rule for the MC-update:

$$W(x'|x) = \frac{e^{-0.5\beta(E_{x'}-E_x)}}{e^{0.5\beta(E_{x'}-E_x)} + e^{-0.5\beta(E_{x'}-E_x)}} \quad (1)$$

You can either write your own program or adapt the provided C template.

b) With the program calculate and plot the magnetization  $\langle |M| \rangle$  as a function of temperature for different system sizes  $L$ .

c) Calculate the Binder cumulant as a function of temperature for different system sizes and estimate the critical temperature.

You can explore your own paths beyond:

For example, determining critical exponents, exploring other boundary conditions, plotting typical Monte Carlo spin configuration for different temperatures, use other lattices, other dimensions ...