University of Göttingen
Institute for Theoretical Physics
Methods of Computational Physics, WiSe 2022/23
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Project 2: Ising model

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1. 1D Ising model (20 points)

Write a program that implements the Metropolis algorithm for single spin flips in a 1D Ising model of N spins producing a new spin configuration X_{k+1} from the present spin configuration X_k. Use the canonical ensemble for a heat bath of temperature T. Set up periodic boundary conditions (effectively bending the chain into circle, such that the first and the last spin are adjacent to each other). Choose units such that $J = 1$. The thermal energy $k_B T$ is given in units of J.

a) Set $N = 20$, and $k_B T = 1$ and simulate $L = 500$ individual trial spin flips. Begin from a "cold" initial state, where all spins are pointing to the same direction. Set the external magnetic field to $H = 0$. Visualise how the spin configuration changes with the number of trial spin flips (i.e. with time). It might be advantageous for the visualisation to show the configuration only after every 5th trial or so. What can you observe? (4 points)

b) Repeat the same simulation for three different thermal energies $k_B T = 0.1$, 1 and 10 and keep track of the energy E at each trial spin flip. For a given configuration $X = \{s_1, \dots, s_N\}$, it is given by

$$E = -J \sum_{i=1}^{N} s_i s_{i+1},$$

with $s_{N+1} = s_1$ due to the periodic boundary condition. Note that we still assume $H = 0$ here, such that the terms involving the interaction with the external field are omitted here.

First run the simulation for at least $L = 1000$ trial spin flips. Plot the time evolution of the energy for each temperature. Your result will be strongly fluctuating. Improve it by repeating each simulation $M = 100$ times, each time starting with a different random seed. Then plot the time evolution of the mean energy $\langle E \rangle$ and its Monte Carlo error estimate $\sqrt{(\langle E^2 \rangle - \langle E \rangle^2)/M}$.

Discuss your result. When is equilibrium reached? What can you observe after the system has reached equilibrium? (4 points)

c) Make a plot of the mean energy per particle $\frac{1}{N}\langle E\rangle_t$ (averaged over simulation time t, e.g. over $L = 1000$ trial spin flips) versus the thermal energy k_BT after equilibrium has been reached (i.e. ignoring the first $L \sim 1000$ trial spin flips). Choose $k_BT = 1\ldots 10$ and average over $M = 100$ independent simulations to obtain a smooth result. Compare to the analytical result for the thermodynamic limit:

$$\frac{E}{N} = -J\tanh\frac{J}{k_BT} = -J\frac{e^{J/k_BT} - e^{-J/k_BT}}{e^{J/k_BT} + e^{-J/k_BT}} = \begin{cases} -J & k_BT \to 0 \\ 0 & k_BT \to \infty \end{cases},$$

and discuss your results. (4 points)

d) Make a plot of the specific heat per particle at constant volume $c_V = \frac{1}{N}C_V$ versus the thermal energy k_BT after equilibrium has been reached. Use the same parameters as in c). As discussed in the lecture, you can calculate C_V as follows:

$$C_V = \frac{\langle E^2\rangle - \langle E\rangle^2}{k_BT^2}$$

Compare to the analytical result for the thermodynamic limit:

$$c_V(k_BT) = k_B\frac{(J/k_BT)^2}{\cosh^2(J/k_BT)},$$

and discuss your results. (4 points)

e) Finally, make a plot of the magnetisation per particle $m = \frac{1}{N}\langle M\rangle$ versus the thermal energy k_BT after equilibrium has been reached. Use the same parameters as in c), but repeat your measurement for different external magnetic fields $H = 0$, 0.1, 1 and 10. For a given configuration X, the magnetisation M is given by

$$M = \sum_{i=1}^{N} s_i.$$

Compare to the analytical result for the thermodynamic limit:

$$m(k_BT) = \frac{e^{J/k_BT}\sinh(H/k_BT)}{\sqrt{e^{2J/k_BT}\sinh^2(H/k_BT) + e^{-2J/k_BT}}},$$

and discuss your results. (4 points)

f) **(Bonus)** A domain is a region of d adjacent spins that all point into the same direction. Make a plot of the average number of domains $\langle n_{\text{domains}}\rangle$ versus the thermal energy k_BT, after equilibrium has been reached. Use the same parameters as in c), Discuss your result. (4 bonus points)

2. 2D Ising model (8 points)

While the 1D Ising model does not yet feature a phase transition, the 2D Ising model already does. This can be seen e.g. in the analytical result for the absolute magnetisation per particle for $H = 0$:

$$|m(T)| = \begin{cases} 0 & : \quad T > T_c \quad k_B T_c \simeq 2.269185J \\ \frac{\left(1+z^2\right)^{1/4}\left(1-6z^2+z^4\right)^{1/8}}{\sqrt{1-z^2}} & : \quad T < T_c \quad\quad z = e^{-2J/k_B T} \end{cases},$$

where T_c is the Curie temperature at which the phase transition occurs.

Implement a 2D Ising model on a square lattice with $n = \sqrt{N} = 30$ spins per side, again using periodic boundary conditions, $s_{n+1,j} = s_{1,j}$ and $s_{i,n+1} = s_{i,1}$, connecting opposite sides with each other. Calculate the absolute magnetisation of the model for $H = 0$ in dependence of the thermal energy $k_B T$ with the same techniques used for the 1D model. Note that more time might be needed to reach equilibrium. Discuss your results. Can you reproduce the predicted phase transition?

3. Bonus: Wang–Landau Sampling

Download the original paper on the Wang-Landau algorithm from Stud.IP ▸ Übung: Methods of Computational Physics ▸ Files ▸ Additional Material. Read it and answer the following questions:

a) **(Bonus)** Does the WLS-Algorithm satisfy Detailed Balance? Comment on the size of possible violations. (2 bonus points)

b) **(Bonus)** To obtain the absolute density of states the numerically determined relative density needs to be normalised. Quote two independent normalisation constraints that can be used for that purpose. (2 bonus points)

c) **(Bonus)** Quote a practical solution to quantify the 'flatness' of the energy density histogram on the fly. (2 bonus points)