Computational Physics SuSe 2023
10. Exercise Sheet

Handing out: 26.06.2023 Prof. H. Jelger Risselada
Submission: 07.07.2023 8 pm

Exercise 0: Comprehension questions 0 Points

1) What is the difference between molecular dynamics (MD) simulation and Monte Carlo (MC) simulation for molecular systems? When is each method suitable?

2) What are the fundamental properties of a Markov process?

Exercise 1: Monte Carlo Simulation of a Single Spin 10 Points

Simulate a single spin $\sigma = \pm 1$ using the Metropolis algorithm with the energy

$$\mathcal{H} = -\sigma H$$

in an external magnetic field H. In the Metropolis algorithm, offer spin flips $\sigma \to -\sigma$.
Numerically calculate the magnetization m at $k_\mathrm{B}T = 1$. In other words, perform Monte Carlo simulations for at least 10^4 values of $H \in [-5, 5]$, each with 10^5 steps, and compare your numerical results with the analytical result

$$m = \tanh(\beta H).$$

Exercise 2: Two-Dimensional Ising Model 30 Points

Simulate the two-dimensional Ising model without a magnetic field using the Metropolis algorithm, with the energy given by

$$\mathcal{H} = -\sum_{i,j \text{ n.n.}} \sigma_i \sigma_j \,,$$

where the sum is taken over nearest neighbors (n.n.). Use a square lattice of size 100×100 with periodic boundary conditions. (If there are issues with computation time, the lattice can be slightly reduced.)
Offer spin flips of randomly selected spins in the Metropolis algorithm. Choose randomly oriented spins or completely ordered spins as initial conditions. After a sufficiently long equilibration phase, perform 10^4 to 10^5 sweeps, where on average each spin is offered a flip once.

1. Generate and discuss graphical snapshots of the system for $k_\mathrm{B}T = 1$ and $k_\mathrm{B}T = 3$.

Consider multiple temperatures $k_\mathrm{B}T \in [1.5, 3]$ for the following parts of the exercise. The range around the critical temperature (in the thermodynamic limit)

$$k_\mathrm{B}T_\mathrm{c} = \frac{2}{\ln\left(1+\sqrt{2}\right)} \approx 2.27$$

is particularly interesting, so it is recommended to resolve the temperature more precisely in this range. For parts of the exercise where plots as a function of time are required, it is sufficient to create plots for the two boundary values of the temperature range and for an intermediate value.

2. First, examine the equilibration phase by measuring the average energy per spin

$$e(t) = \frac{E(t)}{N} = \frac{\langle \mathcal{H}(t) \rangle}{N}$$

as a function of simulation time t, where N is the total number of spins. How long do you have to wait until the result becomes independent of the initial conditions? Examine both initial conditions.

3. Next, consider the time after equilibration. Calculate the averages of the energy, the magnetization

$$\langle m \rangle = \left\langle \frac{1}{N} \sum_i \sigma_i \right\rangle$$

and the absolute value of the magnetization

$$\langle |m| \rangle = \left\langle \frac{1}{N} \left| \sum_i \sigma_i \right| \right\rangle$$

per spin. How does the behavior of the system differ above and below T_c? How does the magnetization $\langle m \rangle(t)$ behave as a function of simulation time at different temperatures?

4. In your simulation, calculate the specific heat per spin from the energy fluctuations

$$c(T) = \frac{\langle \mathcal{H}^2 \rangle - \langle \mathcal{H} \rangle^2}{k_\mathrm{B} T^2 N} \,.$$