ETH
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Optimization & Physics
Exercise 1

HS 07
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The goal of this exercise is to create a framework to test different optimization algorithms.

Problem 1.1 Warm up: The two-dimensional Ising model

As a first step, you are required to write a program to simulate the two-dimensional Ising model on a square lattice using simple Monte Carlo:

$$\mathcal{H} = \sum_{\langle ij \rangle} J_{ij} S_i S_j. \tag{1}$$

In order to be able to test algorithms, make sure that the bonds are not hard-coded (as you would otherwise do for speed) but actually a graph which you can read in from a file or generate with some routine (the file format will be given later in a next exercise). Furthermore, make sure the "engine" (for example Monte Carlo updates, simulated annealing, ...) can be exchanged easily such that you can switch between algorithms. Please us a good RNG such as the Mersenne Twister or r1279 (both available via boost libraries or GSL). Make sure your program measures the energy per spin $\langle E \rangle / N$ and the squared magnetization $\langle m^2 \rangle$, where

$$m = \frac{1}{N} \sum_{i=1}^{N} S_i \tag{2}$$

and $N = L \times L$ is the number of spins for a temperature $T = 0.5$. Note that $\langle \cdots \rangle$ represents a thermal average. For a system of size $L = 8$ plot the energy and the magnetization squared as a function of Monte Carlo time. Make sure you start with a random spin configuration. Print the data in logarithmic spacings ($\tau = 2, 4, 8, 16, \ldots$) such that the figures are not too crowded. To do a quick and dirty estimate of the error bars, simply average the results over several runs (this will come in handy in the next ecercise).

Problem 1.2 The two-dimensional Edwards-Anderson Ising spin glass

Generalize the Ising model previosuly simulated to the two-dimensional Edwards-Anderson Ising spin glass. The code basically remains the same, but you will have to do the following three changes: First, the interactions J_{ij} are now Gaussian distributed with zero mean and standard deviation unity: $\mathcal{P}(J_{ij}) \sim \exp(-J_{ij}^2/2)$. To obtain the Gaussian random numbers, use the Box-Muller method (see Numerical Recipes, or use a library). Because the average magnetization squared in a spin glass is zero, to test equilibration as in the previous problem you will have to simulate the Edwards-Anderson order parameter q defined via

$$q = \frac{1}{N} \sum_{i=1}^{N} S_i^1 S_i^2. \tag{3}$$

To calculate $\langle q^2 \rangle$ you will have to simulate *two* copies $\{S_i^1\}$ and $\{S_i^2\}$ of the system with the *same* disoder, but running on *different* Markov chains, i.e., different initial spin configuration and different sequence of random numbers. As in the previous exercise, study a system of 8×8 spins for $T = 0.5$. Finally, because we want results which do not depend on the choice of the disorder, you will have to average your results over different choices of the disorder, i.e., repeat the calculation above 1000 times and compute $[\langle q^2 \rangle]_{\rm av}$, where now $[\cdots]_{\rm av}$ represents an average over the disorder. Statistical errors can be estimated from

the disorder average (jackknive), whereas the error due to the thermal average can be neglected. How do the equilibration times change in comparison to the previous problem?