Exercises for Computational Physics (physik760)
WS 2017/2018

B. Kostrzewa, M. Petschlies and C. Urbach

---

1 Simulation of the Ising model in two dimensions

Our aim in this CP lecture's tutorial series is two-fold:

1. to practice the mathematical and statistical techniques presented in the lecture
2. to continuously develop your very own toolset for data generation and analysis in Computational Physics

Our first step on this way is the Ising model in two dimensions. As we will see, it is a great testbed for applying and observing many of the techniques and phenomena in Computational Physics.

1.1 The model

Consider a 2-dimensional rectangular lattice $\mathbb{L}$ of $L_\sigma \times L_\tau$ lattice sites. To each site $x \in \mathbb{L}$ we attach a spin variable $s_x \in \{\pm 1\}$. One specific choice of a spin for each lattice site we call a spin configuration $s = \{s_x \,:\, x \in \mathbb{L}\}$.

This system of spins is immersed in a heat bath of constant temperature T and its dynamics are governed by the Hamiltonian

$$\mathcal{H}(s) = -J \sum_{\langle x,y \rangle} s_x\, s_y \,. \tag{1}$$

$\langle x, y \rangle$ denotes the nearest-neighbour pair x and y on the lattice, J is a real number and we assume periodic boundary conditions. In the heat bath environment the probability for finding the spin system at spin configuration s is given by the Boltzmann distribution

$$\mathrm{P}\,(s) = \exp\left(-\frac{\mathcal{H}(s)}{k_B T}\right) / \sum_{s'} \exp\left(-\frac{\mathcal{H}(s')}{k_B T}\right) \,. \tag{2}$$

1: Discuss the physical meaning of J, in particular the sign of J.

2: Formulate in detail the condition for two sites x and y to be nearest neighbours on $\mathbb{L}$, especially with respect to the boundaries.

3: Generate a configuration with randomly arranged spin variables and implement the functional $\mathcal{H}$ to calculate the energy for a given spin configuration. Design appropriate data structures and keep in mind that you will be asked to extend your code in the future, a modular approach is thus recommended.

2 Setting up a development environment

Most of you will be familiar with the Linux environments that are used for the *physik131* EDV course. Because *physik760* heavily uses a number of open-source packages we would like to **strongly** encourage you to use Linux for the tutorials. Not only is a Linux environment generally a good choice as a development platform, doing so will also prevent a number of issues that we have seen in the past. It will also allow you to familarise yourselves with the kind of environment that you are likely to encounter in the future.

For those of you participating on your laptops (rather than the CIP machines in the AVZ), one of our tutors (Martin Ueding) has prepared an *appliance* for the virtual machine *Virtualbox*, which will allow you to run Linux on your Windows machine or Mac. Head over to `http://bulk.martin-ueding.de/cp/readme.html` and follow the instructions to first install Virtualbox and then the appliance.

2.1 Code sharing via github

In order for us to be able to follow your developments, such that we're able to help if and where necessary, we would like you to set up github[1] accounts with the help of your tutors.

You will also need to set up SSH keys on your machines (or inside your virtual machine). After you have set up your accounts and SSH keys, please let your tutors know your account names. One of us (Bartosz Kostrzewa) will then set up private repositories on github to which you will be asked to upload your work. If some of you wish to work as a team, you may also share a single github repository (you may still want to create individual accounts, however).

If you're unfamiliar with git as a version control tool, we have prepared a short introduction (slides and a handout which explains them, as well as exercises) to get you started. See `https://ecampus.uni-bonn.de/goto_ecampus_fold_1105055.html`. There, we also provide links to *cheat sheets*, short references documenting the most common git commands.

[1] `https://www.github.com`