

## Introduction to numerical projects

Here follows a brief recipe and recommendation on how to write a report for each project.

- Give a short description of the nature of the problem and the eventual numerical methods you have used.
- Describe the algorithm you have used and/or developed. Here you may find it convenient to use pseudocoding. In many cases you can describe the algorithm in the program itself.
- Include the source code of your program. Comment your program properly.
- If possible, try to find analytic solutions, or known limits in order to test your program when developing the code.
- Include your results either in figure form or in a table. Remember to label your results. All tables and figures should have relevant captions and labels on the axes.
- Try to evaluate the reliability and numerical stability/precision of your results. If possible, include a qualitative and/or quantitative discussion of the numerical stability, eventual loss of precision etc.
- Try to give an interpretation of your results in your answers to the problems.
- Critique: if possible include your comments and reflections about the exercise, whether you felt you learnt something, ideas for improvements and other thoughts you've made when solving the exercise. We wish to keep this course at the interactive level and your comments can help us improve it.
- Try to establish a practice where you log your work at the computerlab. You may find such a logbook very handy at later stages in your work, especially when you don't properly remember what a previous test version of your program did. Here you could also record the time spent on solving the exercise, various algorithms you may have tested or other topics which you feel worthy of mentioning.
- You should include tests of your algorithms. This could be represented by unit tests and/or tests of mathematical aspects of the algorithm.

## Format for electronic delivery of report and programs

The preferred format for the report is a PDF file. You can also use DOC or postscript formats or as an ipython notebook file. As programming language we prefer that you choose between C/C++, Fortran2008 or Python. The following prescription should be followed when preparing the report:

- Use your github address to hand in your projects.
- Make a folder for each project. For each project you should have three folders: one for the code files, one for the report and finally a folder with specific benchmark calculations. The latter can be in the form of output from your code for a selected set of runs and input parameters.

Finally, we encourage you to work two and two together. Optimal working groups consist of 2-3 students. You can then hand in a common report.

## Project 4, numerical integration, deadline April 29

The project deals with the Ising model in two dimensions, without an external magnetic field. In its simplest form the energy is expressed as

$$E = -J \sum_{\langle kl \rangle}^N s_k s_l \quad (1)$$

with  $s_k = \pm 1$ ,  $N$  is the total number of spins and  $J$  is a coupling constant expressing the strength of the interaction between neighboring spins. The symbol  $\langle kl \rangle$  indicates that we sum over nearest neighbors only. We will assume that we have a ferromagnetic ordering, viz  $J > 0$ . We will use periodic boundary conditions and the Metropolis algorithm only.

- a) Assume we have only two spins in each dimension, that is  $L = 2$ . Find the closed form expression for the partition function and the corresponding expectations values for  $E$ ,  $|\mathcal{M}|$ , the specific heat  $C_V$  and the susceptibility  $\chi$  as functions of  $T$  using periodic boundary conditions.
- b) Write now a code for the Ising model which computes the mean energy  $E$ , mean magnetization  $|\mathcal{M}|$ , the specific heat  $C_V$  and the susceptibility  $\chi$  as functions of  $T$  using periodic boundary conditions for  $L = 2$  in the  $x$  and  $y$  directions. Compare your results with the expressions from a) for a temperature  $T = 1.0$  (in units of  $kT/J$ ).

How many Monte Carlo cycles do you need in order to achieve a good agreement?

- c) We choose now a square lattice with  $L = 20$  spins in the  $x$  and  $y$  directions.

In [b) we did not study carefully how many Monte Carlo cycles were needed in order to reach the most likely state. Here we want to perform a study of the time (here it corresponds to the number of Monte Carlo cycles) one needs before one reaches an equilibrium situation and can start computing various expectations values. Our first attempt is a rough and plain graphical one, where we plot various expectations values as functions of the number of Monte Carlo cycles.

Choose first a temperature of  $T = 1.0$  (in units of  $kT/J$ ) and study the mean energy and magnetisation (absolute value) as functions of the number of Monte Carlo cycles. Use both an ordered (all spins pointing in one direction) and a random spin orientation as starting configuration. How many Monte Carlo cycles do you need before you reach an equilibrium situation? Repeat this analysis for  $T = 2.4$ .

Make also a plot of the total number of accepted configurations as function of the total number of Monte Carlo cycles. How does the number of accepted configurations behave as function of temperature  $T$ ?

- d) Compute thereafter the probability  $P(E)$  for the previous system with  $L = 20$  and the same temperatures. You compute this probability by simply counting the number of times a given energy appears in your computation. Start the computation after the steady state situation has been reached. Compare your results with the computed variance in energy  $\sigma_E^2$  and discuss the behavior you observe.

Near  $T_C$  we can characterize the behavior of many physical quantities by a power law behavior. As an example the mean magnetization is given by

$$\langle \mathcal{M}(T) \rangle \sim (T - T_C)^\beta, \quad (2)$$

where  $\beta = 1/8$  is a so-called critical exponent. A similar relation applies to the heat capacity

$$C_V(T) \sim |T_C - T|^\alpha, \quad (3)$$

and the susceptibility

$$\chi(T) \sim |T_C - T|^\gamma, \quad (4)$$

with  $\alpha = 0$  and  $\gamma = 7/4$ . Another important quantity is the correlation length, which is expected to be of the order of the lattice spacing for  $T \gg T_C$ . Because the spins become more and more correlated as  $T$  approaches  $T_C$ , the correlation length increases as we get closer to the critical temperature. The divergent behavior of  $\xi$  near  $T_C$  is

$$\xi(T) \sim |T_C - T|^{-\nu}. \quad (5)$$

A second-order phase transition is characterized by a correlation length which spans the whole system. Since we are always limited to a finite lattice,  $\xi$  will be proportional with the size of the lattice. Through so-called finite size scaling relations it is possible to relate the behavior at finite lattices with the results for an infinitely large lattice. The critical temperature scales then as

$$T_C(L) - T_C(L = \infty) = aL^{-1/\nu}, \quad (6)$$

with  $a$  a constant and  $\nu$  defined in Eq. (??). We set  $T = T_C$  and obtain a mean magnetisation

$$\langle \mathcal{M}(T) \rangle \sim (T - T_C)^\beta \rightarrow L^{-\beta/\nu}, \quad (7)$$

a heat capacity

$$C_V(T) \sim |T_C - T|^{-\gamma} \rightarrow L^{\alpha/\nu}, \quad (8)$$

and susceptibility

$$\chi(T) \sim |T_C - T|^{-\alpha} \rightarrow L^{\gamma/\nu}. \quad (9)$$

- e) We wish to study the behavior of the Ising model in two dimensions close to the critical temperature as a function of the lattice size  $L \times L$ . Calculate the expectation values for  $\langle E \rangle$  and  $\langle |\mathcal{M}| \rangle$ , the specific heat  $C_V$  and the susceptibility  $\chi$  as functions of  $T$  for  $L = 20, L = 40, L = 60$  and  $L = 80$  for  $T \in [2.0, 2.4]$  with a step in temperature  $\Delta T = 0.05$  or smaller. Plot  $\langle E \rangle$ ,  $\langle |\mathcal{M}| \rangle$ ,  $C_V$  and  $\chi$  as functions of  $T$ . Can you see an indication of a phase transition?

Use the absolute value  $\langle |\mathcal{M}| \rangle$  when you evaluate  $\chi$ .

- f) Use Eq. (??) and the exact result  $\nu = 1$  in order to estimate  $T_C$  in the thermodynamic limit  $L \rightarrow \infty$  using your simulations with  $L = 20, L = 40, L = 60$  and  $L = 80$ . The exact result for the critical temperature (after Lars Onsager) is  $kT_C/J = 2/\ln(1 + \sqrt{2}) \approx 2.269$  with  $\nu = 1$ .

## Background literature

If you wish to read more about the Ising model and statistical physics here are two suggestions.

1. M. Plischke and B. Bergersen, Equilibrium Statistical Physics, Prentice-Hall, see chapters 5 and 6.
2. M. E. J. Newman and T. Barkema, Monte Carlo methods in statistical physics, Oxford, see chapters 3 and 4.