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 reliabilty 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 you 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.

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. As programming language we prefer that you choose between C/C++ and Fortran90/95. You could also use Java or Python as programming languages. Matlab/Maple/Mathematica/IDL are not allowed as programming languages for the handins, but you can use them to check your results where possible. The following prescription should be followed when preparing the report:

- Use Classfronter to hand in your projects, log in at blyant.uio.no and choose 'fellesrom fys3150 og fys4150'. Thereafter you will see an icon to the left with 'hand in' or 'innlevering'. Click on that icon and go to the given project. There you can load up the files within the deadline.

- Upload **only** the report file and the source code file(s) you have developed. The report file should include all of your discussions and a list of the codes you have developed. Do not include library files which are available at the course homepage, unless you have made specific changes to them.

- Comments from us on your projects, approval or not, corrections to be made etc can be found under your Classfronter domain and are only visible to you and the teachers of the course.

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

Project 4, Potts model in two dimensions, deadline 31 october 12pm (midnight)

For this project you can build upon program programs/chapter10/ising_2dim.cpp (or the f90 version).

The Potts model has been, in addition to the Ising model, widely used in studies of phase transitions in statistical physics. The so-called two-dimensional q-state Potts model has an energy given by

$$E = -J \sum_{<kl>}^{N} \delta_{s_l,s_k},$$

where the spin s_k at lattice position k can take the values $1, 2, \ldots, q$. The Kroneckr delta function δ_{s_l,s_k} equals unity if the spins are equal and is zero otherwise. N is the total number of spins. For $q = 2$ the Potts model corresponds to the Ising model. To see that we can rewrite the last equation as

$$E = -\frac{J}{2} \sum_{<kl>}^{N} 2(\delta_{s_l,s_k} - \frac{1}{2}) - \sum_{<kl>}^{N} \frac{J}{2}.$$

Now, $2(\delta_{s_l,s_k} - \frac{1}{2})$ is $+1$ when $s_l = s_k$ and -1 when they are different. This model is thus equivalent to the Ising model except a trivial difference in the energy minimum given by a an additional constant and a factor $J \rightarrow J/2$. One of the many applications of the Potts model is to helium absorbed on the surface of graphite.

The Potts model exhibits a second order phase transition for low values of q and a first order transition for larger values of q. Using Eherenfest's definition of a phase transition, a second order phase transition has second derivatives of the free energy that diverge

(the heat capacity and susceptibility in our case) while a first order transition has first derivatives like the mean energy that diverge. Since the calculations are done with a finite lattice it is always difficult to find the order of the phase transitions. In this project we will limit ourselves to find the temperature region where a phase transition occurs and see if the numerics allow us to extract enough information about the order of the transition.

a) Write a program which simulates the $q = 2$ Potts model for two-dimensional lattices with 10×10, 40×40 and 80×80 spins and compute the average energy and specific heat. Compute also the absolute value of the mean magnetization and the susceptibility. Establish an appropriate temperature range for where you see a sudden change in the heat capacity and susceptibility. To get appropriate statistics you should allow for at least 10^5 Monte Carlo cycles. In setting up this code you need to find an effecient way to simulate the energy differences between different microstates.

b) Compare these results with those obtained with the two-dimensional Ising model. The exact critical temperature for the Ising model is $T_C = 2.269$. Here you can eventually use the abovementioned program from the lectures or write your own code for the Ising model.

c) Extend the calculations to the Potts model with $q = 3, 6$ and $q = 10$. Make a table of the possible values of ΔE for each value of q. Establish first the location of the peak in the specific heat and study the behavior of the mean energy and magnetization as functions of q. Do you see a noteworthy change in behavior from the $q = 2$ case? For larger q values you may need lattices of at least 50×50 in size.