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 accepted, but you can use them to check your results where possible. Finally, we do prefer that you work together. Optimal working groups consist of 2-3 students, but more people can collaborate. You can then hand in a common report.

Project 1, Phase transitions in spin systems using the Potts Model, deadline march 5 12am (midnight)

For this project you can build upon the programs for the Ising model and the Potts model on the webpage of the course, see the programs link. For a discussion of the Potts models, see chapter 4.5 of Barkema and Newman.

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 Kronecker 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 $J \to J/2$. 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 or are discontinuous (the heat capacity and susceptibility in our case) while a first order transition has first derivatives like the mean energy that are discontinuous.

a) Write a program which simulates the $q = 2$ Potts model for a two-dimensional lattice with 40×40 spins and compute the average energy and specific heat. Compute also the absolute value of the mean magnetization, the susceptibility and the correlation function

$$G_{ij} = \langle s_i s_j \rangle - \langle s_i \rangle \langle s_j \rangle. \tag{1}$$

(See Eq. (3.50) in the text of Barkema and Newman). 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 10^6 Monte Carlo cycles. In setting up this code you need to find an effecient way to simulate the energy differences between different microstates.

In the first part of this project we limit ourselves to the Metropolis algorithm.

Compare these results with those obtained with the two-dimensional Ising model. The exact critical temperature for the Ising model is $T_C = 2.269$. For the Potts

model with $q = 2$ it is half this value. For the Ising model you can use the program from the lectures or write your own code for the Ising model.

b) Here we study the time autocorrelation function, defined by Eq. (3.21) from the text of Newman and Barkema. We use again the square lattice with $L = 40$ spins in the x and y directions. Choose first a temperature below the assumed critical temperature (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 or have the same value) and a random spin orientation as starting configuration. How many Monte Carlo cycles do you need before you reach an equilibrium situation? Can you extract an equilibration measure? Repeat this analysis for a temperature above the critical . Try also different seeds for the random number generators. The evaluation of the autocorrelation function should be included in all your further calculations.

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

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

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

$$C_V(T) \sim |T_C - T|^{\alpha}, \tag{3}$$

and the susceptibility

$$\chi(T) \sim |T_C - T|^{\gamma}, \tag{4}$$

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 $T >> T_C$. 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 ξ near T_C is

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

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, ξ will be proportional with the size of the lattice. Through finite size scaling relations, see chapter 8.3 of Newman and Barkema, it is possible to relate the behavior at finite lattices with the results for an infinitely large lattice. The critical temperature scales then as

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

with a a constant and ν defined in Eq. (5). The correlation length is given by

$$\xi(T) \sim L \sim |T_C - T|^{-\nu}. \tag{7}$$

and if we set $T = T_C$ one obtains

$$\langle \mathcal{M}(T) \rangle \sim (T - T_C)^{\beta} \rightarrow L^{-\beta/\nu}, \tag{8}$$

a heat capacity

$$C_V(T) \sim |T_C - T|^{-\gamma} \rightarrow L^{\alpha/\nu}, \tag{9}$$

and susceptibility

$$\chi(T) \sim |T_C - T|^{-\alpha} \rightarrow L^{\gamma/\nu}. \tag{10}$$

For all productions runs, you should parallelize the code at this stage. When doing this, be sure that you obtain the same results as with the serial code.

c) We will now study the behavior of the $q = 2$ Potts model in two dimensions close to the critical temperature as a function of the lattice size L. Calculate the expectation values for $\langle E \rangle$ and $|\langle \mathcal{M} \rangle|$, the specific heat C_V, the susceptibility χ and the correlation function $G(r)$ as functions of T for $L = 20$, $L = 40$, $L = 60$, $L = 80$ and $L = 100$ for T near the critical temperature $T_C \approx 1.1345$ for small temperature steps $\Delta T = 0.01 - 0.05$. Plot $\langle E \rangle$, $\langle \mathcal{M} \rangle$, C_V and $G(r)$ as functions of T. Can you see an indication of a phase transition? Try to extract the correlation length ξ from the formal definition of the correlation function

$$\xi^{-1} = -\lim_{r \rightarrow \infty} \frac{\partial}{\partial r} lnG(r), \tag{11}$$

with $r = |i - j|$.

d) Use Eq. (6) and the exact result $\nu = 1$ in order to estimate T_C in the thermodynamic limit $L \rightarrow \infty$ using your simulations with $L = 20$, $L = 40$, $L = 60$, $L = 80$ and $L = 100$.

e) We use the exact result $kT_C/J = 1/ln(1 + \sqrt{2}) \approx 1.1345$ and $\nu = 1$. Determine the numerical values of C_V, χ and $\mathcal{M}$ at the exact value $T = T_C$ for $L = 20$, $L = 40$, $L = 60$, $L = 80$ and $L = 100$. Plot $log_{10}(\mathcal{M})$ and $log_{10}(\chi\ log_{10})$ as functions of $log_{10}(L)$ and use the scaling relations of Eqs. (8) and (10) in order to determine the constants β and γ. Are your log-log plots close to straight lines? The exact values are $\beta = 1/8$ and $\gamma = 7/4$. Can you extract a behavior for the correlation function?

f) Use the exact value of T_C and compute the correlation time $\tau \sim L^z$ (Eq. (4.7)) for the above lattices and make a log-log plot as in Figure 4.2 of Newman and Barkema. Comment your results for the Metropolis algorithm.

g) The last result shows that the Metropolis algorithm is inefficient close to the critical temperature. Repeat the analysis of [d-f)] using the Wolff algorithm discussed in chapters 4.2 and 4.3. Discuss your results.

h) Extend the calculations to the Potts model with $q = 3$ and $q = 6$. 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? Here you need only to find a region where you see that these variables change dramatically. These results are simply used for the refined search in the next exercise.

i) We study closer the behavior of the $q = 3, 6$ Potts models in two dimensions close to the critical temperature as a function of the lattice size $L \times L$. Use the Wolff and Metropolis algorithms. Calculate the expectation values for $\langle E \rangle$ and $|\langle \mathcal{M} \rangle|$, the specific heat C_V and the correlation function $G(r)$ as functions of T for $L = 20$, $L = 40$, $L = 60$, $L = 80$ and $L = 100$ for T near the established critical temperature from the previous step. Plot $\langle E \rangle$, $\langle \mathcal{M} \rangle$, C_V and $G(r)$ as functions of T. Can you see an indication of a phase transition? What is its character? Comment your results. Compare your critical temperature with the values from the literature, see for example the references listed below. (If you have time, consider also introducing the Heat-Bath algorithm discussed in chapter 4.5 of Barkema and Newman.)

For a reference on the critical temperatures of the Potts Models, see J. L. Monroe, Physical Review E **66**, 066129 (2002) and http://prola.aps.org/abstract/PRE/v66/i6/e066129. See also Challa and Landau at http://link.aps.org/abstract/PRB/v34/p1841.