Monte Carlo simulation methods **Homework 3, 1.11.2007**

Return the solutions (with program printouts) at the latest at the beginning of the 1.11. excercise session. You can also e-mail the solutions to Ahti Leppänen, <ahtilepp AT mail.student.oulu.fi>.

Potts model is a generalisation of the Ising model. A q-state Potts model in 2 dimensions on a regular square lattice has spins s_i with q different states, $s_i = 1, \ldots, q$, and its action and partition function are

$$S = \beta \sum_{<i,j>} [1 - \delta(s_i, s_j)], \qquad Z = \sum_{\{s_i\}} e^{-S},$$

where the sum goes over nearest-neighbour pairs on a square lattice (once per pair), and $\delta(i, j) = 1$ if $i = j$, 0 otherwise. We assume here periodic boundary conditions. Write a 2-dimensional $q = 3$ -state Potts model simulation program, using heat bath or Metropolis algorithm, for simulations on rectangular $V = L_x \times L_y$ lattices. Measure absolute magnetisation

$$|M| = \frac{3}{2}\left[\max(M_1, M_2, M_3) - \frac{1}{3}\right], \qquad \text{where} \quad M_s = \frac{1}{V}\sum_i \delta(s, s_i),$$

where normalisation is such that $0 \le |M| \le 1$.

Perform a series of simulations on a $\sim 64^2$ lattice in the β-range $0.5 < \beta < 1.5$, at ~ 10 different values of β, and (at least) ~ 30000 update sweeps for each value of β. Calculate $\langle |M| \rangle(\beta)$, with error estimates (remember thermalisation!). Show that the results indicate a phase transition at $\beta = \ln(1 + \sqrt{3}) \approx 1.0051$. Do one simulation at this value of β. Plot $\langle |M| \rangle(\beta)$ and *autocorrelations* of $|M|$ as functions of β.

You can take as your starting point the `ising_sim.c` program on the course web pages. Modifications to it are straightforward.

For error analysis, you can use the `errors.c` program, which also calculates autocorrelation times. Remember to skip the thermalisation at the beginning! The program uses command line arguments to select the data and analysis method. You can get short list of options by issuing only the command name without any options or filenames. More information can be found in the source code.

2-dimensional Potts models have not been exactly solved, but many properties at the critical point are known. For a q-state model the transition happens at $\beta_c = \ln(1 + \sqrt{q})$. If $q \le 4$, the transition is of second order, otherwise first order. In 3 dimensions the transition is of first order except for $q = 2$.