Monte Carlo simulation methods, homework 3

Updating

Quite similar to the way done for Ising model(lectures page 46/ising_sim.c example program). Now the local energy functional needed in update(Heat bath/Metropolis) is

$$S_x(s_x) = \beta \sum_{\text{y=n.n.of x}} [1 - \delta(s_x, s_y)]$$

Metropolis update

Compared to updating Ising model, the difference is that one can't simply 'flip' a spin because there are more than two states, but with 3 states as the trial state one can for example choose one of the two different states randomly with even probability.

Heat bath update

In Ising model, the new state s_x was chosen with probability

$$p(s_x) = \frac{e^{-S_x(s_x)}}{e^{-S_x(+1)} + e^{-S_x(-1)}}$$

where S_x is the local energy functional. Now there's simply one more state, so the probability is

$$p(s_x) = \frac{e^{-S_x(s_x)}}{e^{-S_x(0)} + e^{-S_x(1)} + e^{-S_x(2)}}$$

where indeces 0,1,2 are used to denote different states.

Thermalization

The initial configuration may be 'bad' and the first measurement may thus be simply 'wrong', and should not be taken into account when calculating averages (for example if the initial configuration is totally ordered and the equilibrium configuration is unordered, measurements taken while the system is still ordered are not 'right'). How long it takes for the system to thermalize? Details depends on the problem, but a rule of the thumb is that one should discard at least $n >> \tau$ measurements from the beginning, often values

$$n = 5\tau...10\tau$$

Also, simple plot of the observable as a function of simulation time can give hint about this.

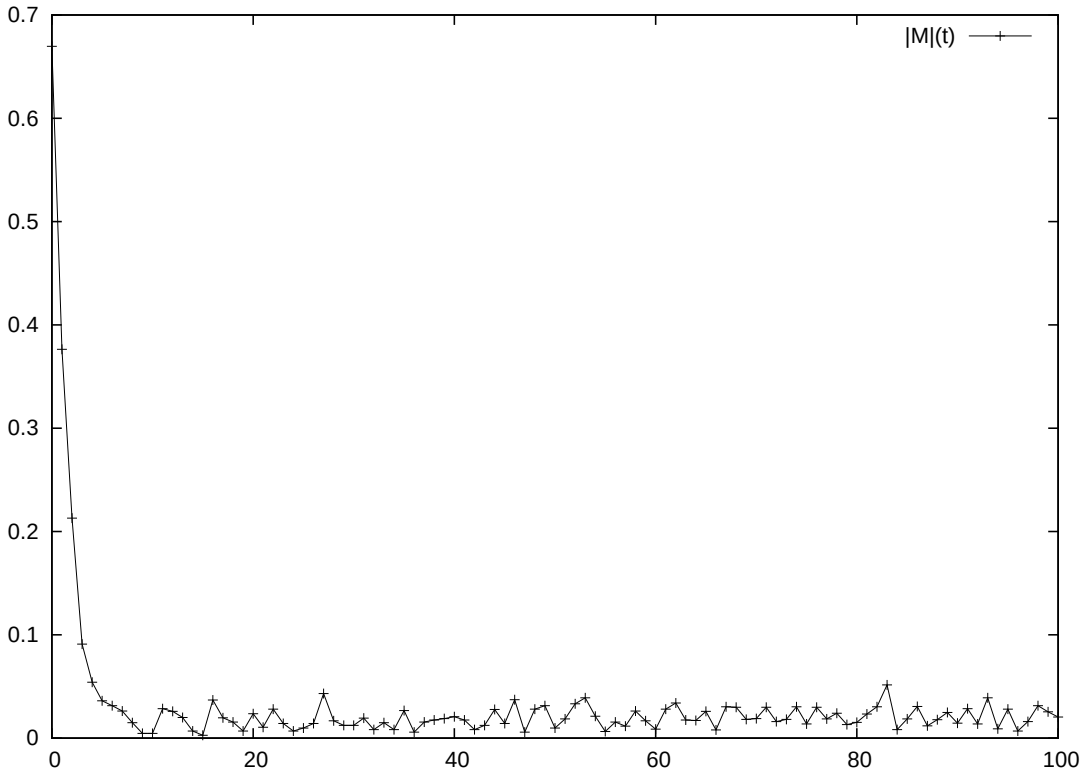

Figure 1: Value of $|M|$ as function of simulation time. Initial configuration was totally ordered($|M| = 1$) and the average obtained by the calculation was ≈ 0.02; so discarding first ten or so measurements seems sufficient.

Results

Implementation

The results presented here were obtained with following implementation:

- Metropolis update with typewriter ordering and periodic boundaries, where trial spin value was chosen randomly from two different states with even probability.
- Simulation time is the same as number of update sweeps done.
- Measurements were done after every sweep and measurement value was written to file.
- Averages and autocorrelation times were then calculated using errors.c available in the courses webpage.
- For thermalization, the autocorrelation times were calculated from the whole data, and then values were recalculated discarding $10 * \tau_{int}$ measurements from the beginning.

β	$< \lvert M \rvert >$	Error estimate	τ_{int}
0.5	0.01831	0.000069	0.67
0.6	0.0212	0.00010	1.1
0.7	0.0258	0.00016	1.8
0.8	0.0345	0.00031	3.7
0.9	0.0544	0.00095	14
1.0051	0.56	0.041	571
1.1	0.9068	0.00033	10
1.2	0.9535	0.00010	3.9
1.3	0.97364	0.000055	2.6
1.4	0.98422	0.000038	2.4

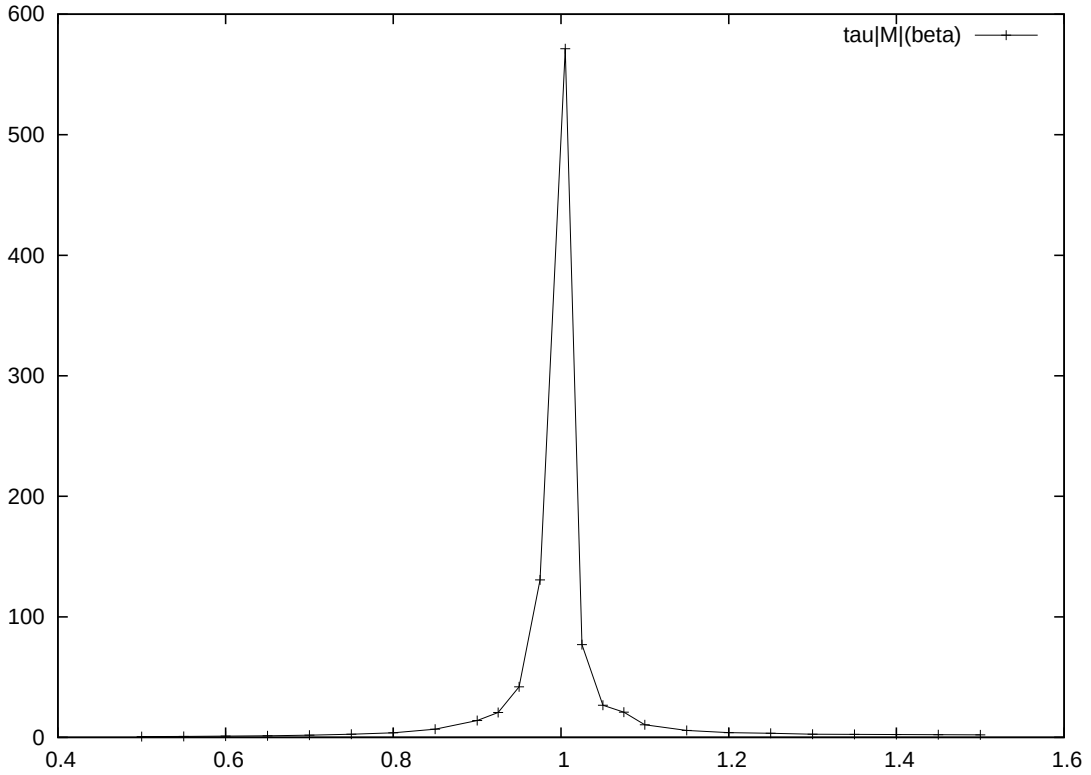

Figure 2: Autocorrelation times as function of β. Note that the autocorrelation time depends for example from 'definition of time'(measurement frequency), update method etc.

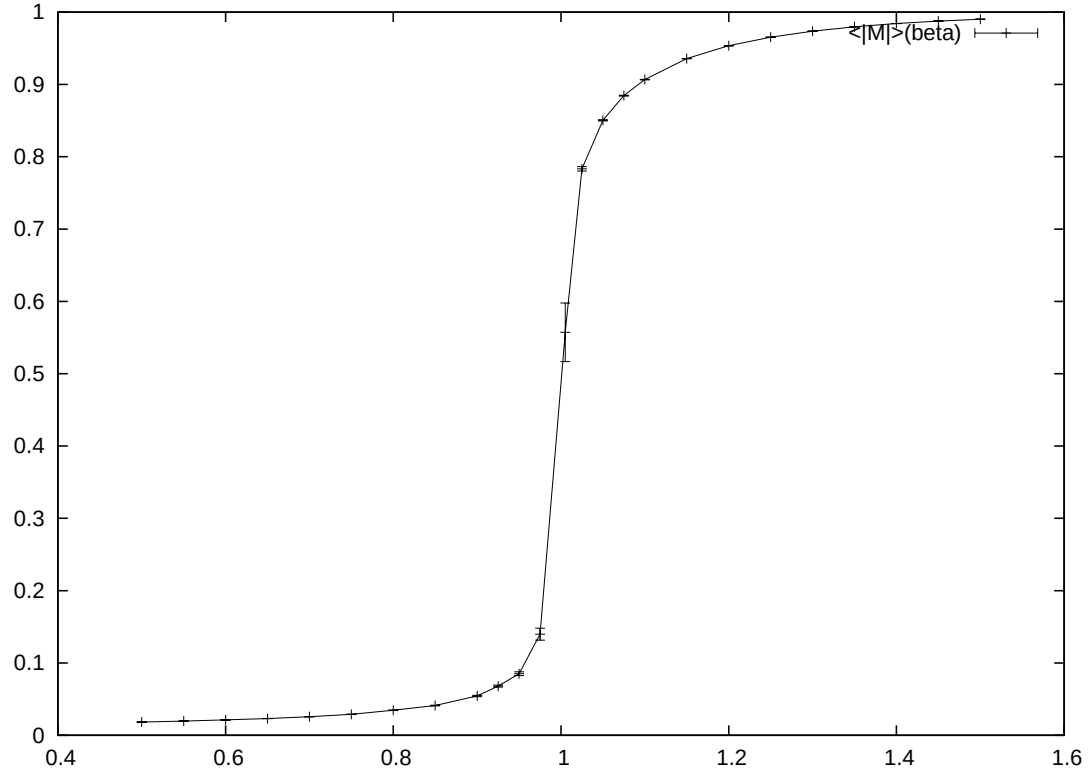

Figure 3: Average of $|M|$ as function of β. The exact phase transition point can't be deducted from these calculations only, but it seems to fit well to the analytic phase transition point ≈ 1.0051