Computational Science 2

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Seminar
Exercises

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Exercise 9 (6.6.2019):

The demon algorithm and the 1D Ising model

from ***An Introduction to Computer Simulation Methods***,
Chapter 15, Problem 15.5-6

a) Write a target class to use with `IsingDemon` and simulate the one-dimensional (1D) Ising model. Choose $N = 100$ and the desired total energy, $E = -20$. Describe qualitatively how the configurations change with time. Then let $E = -100$ and describe any qualitative changes in the configurations.

b) Compute the demon energy E_d and the magnetization M as a function of the time. As usual, we interpret the time as the number of Monte Carlo sweeps, i.e. Monte Carlo steps per spin (mcs). What is the approximate time for these quantities to approach their equilibrium values?

c) Compute the equilibrium values of $\langle E_d \rangle$ and $\langle M^2 \rangle$. About 100 mcs is sufficient for testing the program and yields results of approximately 20% accuracy. To obtain better than 5% results, choose mcs ≥ 1000.

d) Compute T for $N = 100$ and $E = -20, -40, -60$, and -80 from the inverse slope of $P(E_d)$ and the relation

$$kT/J = \frac{4}{\ln(1 + 4J/\langle E_d \rangle)}. \tag{1}$$

Compare your results to the exact result for an infinite one-dimensional lattice, $E/N = -\tanh(J/kT)$. How do your computed results for E/N depend on N and on the number of mcs? Does $\langle M^2 \rangle$ increase or decrease with T?

e) Modify `IsingDemon` to include a nonzero magnetic field and compute $\langle E_d \rangle$, $\langle M \rangle$, and $\langle M^2 \rangle$ as a function of B for fixed E. Determine the relation of $\langle E_d \rangle$ to T for your choices of B. Or determine T from the inverse slope of $P(E_d)$. Is the equilibrium temperature higher or lower than the $B = 0$ case for the same total energy?

f) Modify `IsingDemon` so that the antiferromagnetic case, $J = -1$, is treated. Before doing the simulation, describe how you expect the configurations to differ from the ferromagnetic case. What is the lowest energy or ground state configuration? Run the simulation with the spins initially in their ground state, and compare your results with your expectations. Compute the mean energy per spin versus temperature and compare your results with the ferromagnetic case.