

---

**Becs-114.1100 Computational Science / Laskennallinen tiede. Fall 2015.**

Assignment 10 (the last one). Monte Carlo simulations.

Due Tue 01.12.2015 11 pm.

Extra points are added to the total score for those who otherwise would not get the required minimum of 15 points. Once you reach 15 points, additional extra points do not count.

Web page: <https://mycourses.aalto.fi/course/view.php?id=4367>

*computer* = programming task

*pencil and paper* = solve on paper

---

**Problem 1. (*computer*) (5 points)**

Write a program to perform a Metropolis Monte Carlo simulation of the 2D Ising model in zero field ( $H = 0$ ) and on a square  $L \times L$  lattice. The Hamiltonian of this model is given by

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} s_i s_j \quad (s_{i,j} = \pm 1)$$

where the sum is over all distinct nearest-neighbor pairs and  $s_i$  and  $s_j$  are the values of the spins at the lattice sites  $i$  and  $j$ . Set  $J = 1$ . Use periodic boundary conditions and spin-flip updates. Temperatures are expressed in energy units. Time is expressed in units of Monte Carlo steps (MCS) (1 MCS = 1 update per spin on average, i.e. total of  $L \times L$  random updates).

(a) Check that the ground state energy is calculated correctly. (Use all-spins-up or all-spins-down as your initial configuration and calculate the energy of this configuration.)

For the following, the task is to study the  $32 \times 32$  Ising model at three different temperatures:  $T = 2.1$ , 2.265 and 3.5. Note: the middle temperature  $T = 2.265$  is difficult and the results will look different than for the other two cases.

(b) Estimate a suitable equilibration time for  $T = 2.1$  and 3.5. Perform several short runs and plot the magnetization  $m$  and the internal energy  $u$  per spin as a function of time (in MCS). Use a random spin configuration as your initial state. Remember to use different random number sequences for the separate runs.

(c) For  $T = 2.265$ , perform a long simulation run of at least 50 000 MCS and plot the resulting magnetization curve. Can you explain what is happening? How will the behavior affect the time needed to perform measurements at this temperature?

(d) Show a snapshot of a typical equilibrium configuration for each temperature. (You can plot the lattice for example using the commands `surf()` and `view(2)` in Matlab.)

(e) Compute  $\langle m \rangle$  and  $\langle |m| \rangle$  for each temperature. Calculate the averages over several independent runs starting each run with a random spin configuration (remember to equilibrate the system in the beginning of each run). Explain the results.

**Problem 2. (computer) (1 extra point\*)**

Write a program which performs a simple random walk on a square 2D lattice. Measure the mean squared displacement  $\langle R^2(N) \rangle$  as a function of the number of steps  $N$ . For each value of  $N$ , perform several independent simulations to obtain the value of  $\langle R^2(N) \rangle$ .  $R(N)$  denotes the distance between the initial site and the final site after  $N$  steps.

What relation does  $\langle R^2(N) \rangle$  follow?

**Problem 3. (computer) (3 extra points\*)**

Write a program which performs a simulation of surface diffusion using the lattice gas model on a square  $L \times L$  lattice. In this model, each lattice site is either occupied ( $n_i = 1$ ) or unoccupied ( $n_i = 0$ ) by a particle. Particle concentration is defined as  $\theta = N_p / (L \times L)$  where  $N_p$  is the total number of particles on the lattice. Diffusion is modeled by considering each atom as a random walker. The only interaction between the particles is the exclusion of double occupancy of lattice sites.

(a) Calculate the mean squared displacement of the collection of atoms as a function of time (in MC steps) for varying concentrations of  $\theta = 0.01, 0.1, 0.2, 0.5, 0.8$ . Show a plot of your results.

(b) Using the results obtained in (a), calculate the diffusion constant  $D$  as a function of particle concentration. Show a plot of your results.

Note that the program of problem 2 can be used as a starting point of problem 3.

---

This is the last assignment.

You must obtain at least 15 points overall from the exercises to take the exam. Bonus for the exercise points is converted into exam points with some ratio.

\*) The extra points are ONLY for passing the 15 points limit. They do not add to the exam points.

---