

## Session 2 : importance and Rosenbluth sampling

You can download the computer exercises until the 21st of October 2009 at the address:  
<http://dl.ens-lyon.fr/bigfilesharing/files/6983db25b55421123a118fb30d573c29/prgmS2.zip>

### 1 2D-Ising model

We assume the same formalism than exercise 2 of session 1.

1. Adapt the Metropolis scheme to the present problem. How do you generate the new configuration? (local moves, global moves, random matrix generation?) Compute the free energy difference  $\Delta E$  after a single spin flip.
2. At a given temperature  $T_0$ , during the Metropolis process, we construct the histogram  $\mathcal{N}_0(M, NNC)$  representing how often the system has reached the magnetization  $M$  and the nearest-neighbour coupling  $NNC$ . Think about when update the histogram. How can one compute the thermodynamic average  $\langle X \rangle(T_0)$  of a given variable from  $\mathcal{N}_0(M, NNC)$ ?
3. Evaluate the standard deviation for the estimation of  $\langle X \rangle(T_0)$  after  $N_f$  spin flips.
4. Complete the subroutine *metropolis.f90* to code the Metropolis scheme and choose when update  $\mathcal{N}_0(M, NNC)$ .
5. Compute and trace  $\bar{M}(T_0)$  and  $\mathcal{N}_0(M, NNC)$  for  $T_0 = 1.5, 2, 2.5, 3, 4, 5, 6, 8, 10$ .
6. From a single run at  $T_0$ , how can one estimate the density of state? Remark: try to link  $\mathcal{N}_0(M, NNC)$  and  $D(M, NNC)$ .
7. Complete the subroutine *rsm2.f90* to compute  $\bar{M}(T)$  from  $D$ .
8. Trace the obtained evolutions of  $\bar{M}(T)$  for  $T_0 = 1.5, 2, 2.5, 3, 4, 5, 6, 8, 10$ . Any comments?
9. How can one evaluate the critical temperature using the histograms? Try to estimate  $T_c$ . Compare with the Onsager value.

### 2 Rosenbluth sampling for chain molecules

We use the same lattice and same notations than exercise 3 in session1.

#### 2.1 The method

The Rosenbluth method consists of two steps: a) generate a chain conformation with a bias that ensures that "acceptable" conformations are created with a high probability; b) correct the bias by multiplying with a weight factor. In the Rosenbluth scheme, a conformation is constructed segment by segment. For every segment, we have a choice of  $z$  possible directions. Contrary to simple sampling where the choice is random, the Rosenbluth approach favors the direction with the largest Boltzmann factor. To be more specific, the following scheme is used to generate a configuration of one polymer with  $N + 1$  monomers:

- a) the first monomer is inserted at position  $(0, 0, 0)$ .
- b) for all monomers  $i = 2, 3, \dots, N + 1$ , we consider all  $z$  trial positions adjacent to monomer  $i - 1$ . The energy of the  $j$ th trial position is denoted  $u^i(j)$ . From the  $z$  possibilities, we select one, say  $l$ , with a probability

$$p^i(l) = \frac{\exp(-\beta u^i(l))}{w_i} \quad (1)$$

where

$$w_i = \sum_{j=1}^z \exp(-\beta u^i(j)) \quad (2)$$

The energy  $u^i(j)$  excluded the interactions with the monomers  $i + 1$  to  $N + 1$ . Hence, the total energy of the chain conformation  $\Gamma$  is given by  $U(\Gamma) = \sum_{i=1}^{N+1} u^i(l)$ . By convention  $u^1(j) = 0$  and  $w_1 = 1$ .

- c) Step b) is repeated until the entire chain is grown. Then, we compute the Rosenbluth factor of  $\Gamma$

$$W(\Gamma) = \prod_{i=1}^{N+1} w_i \quad (3)$$

If during the process we find a dead alley (all the neighbors are occupied), we throw out the conformation and begin a new growth from step a).

1. After generating a large number  $P$  of configurations, the ensemble averaged properties are calculated as follows:

$$\langle X \rangle = \frac{\sum_{i=1}^P W(\Gamma_i) \times X(\Gamma_i)}{\sum_{i=1}^P W(\Gamma_i)}. \quad (4)$$

Prove the correctness of this formula. Remark: think about the probability to generate a given conformation.

2. Derive a formula for the error made when evaluating  $\langle X \rangle$ .
3. Show that by taking the average Rosenbluth factor, we get an access to the free energy.
4. Compare with classical importance sampling.

## 2.2 Application to 3D SAW

We apply the Rosenbluth technique to 3D SAW.

1. Complete the subroutine *rosenbluth.f90* to generate conformations with the Rosenbluth scheme and compute its end-to-end distance.
2. Complete the computation of  $\log \mathcal{N}_{SAW}(N)$  and  $R_{rms}(N)$  in *main.f90*.
3. Theoretically, one can show that  $R_{rms}(N) \sim N^c$  and  $\mathcal{N}_{SAW}(N) \sim \mu^N N^{1/6}$ . Evaluate  $c$  and  $\mu$ .
4. What happens for large  $N$  ( $N > 300$ )? Why? Any comments?