

## Problem set 2: Metropolis Criterion, Ising Model

1. a. You have generated 100000 configurations of a Lennard-Jones system using (1) simple sampling, (2) importance sampling. How do you calculate the average energy?

Simple sampling:

$$\frac{\sum_i E_i \cdot \exp(-\beta E_i)}{\sum_i \exp(-\beta E_i)}$$

Importance sampling

$$\frac{1}{N} \sum_i E_i$$

- b. Verify that the Metropolis criterion enforces detailed-balance. (Distinguish between  $\Delta E < 0$  und  $\Delta E > 0$ .)

$\Delta E < 0$  (see handout last lecture)

$\Delta E > 0$ :  $W_{ij} = \exp(-\beta \Delta E)$ ,  $W_{ji} = 1 \rightarrow W_{ij}/W_{ji} = \exp(-\beta \Delta E)$  q.e.d.

- c. The Glauber algorithm has the following acceptance rule:  
 $W_{ij} = (1 - \tanh(\beta(E_j - E_i)/2))$ .  
 Show that this algorithm enforces detailed balance, too.  
 (Hint:  $\tanh(x) = (e^x - e^{-x}) / (e^x + e^{-x})$ .)

$x = \beta \Delta E / 2$

$1 - (e^x - e^{-x}) / (e^x + e^{-x}) / (1 - (e^{-x} - e^x) / (e^{-x} + e^x)) = e^{-2x} = \exp(-\beta \Delta E)$  q.e.d.

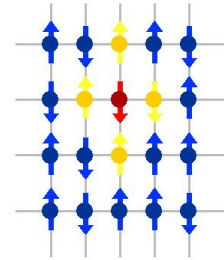
- d. Formulate the Metropolis Criterion for a local displacement in a system of hard discs in the canonical ensemble.

No overlap:  $W_{ij} = 1$ ,

Overlap:  $W_{ij} = \exp(-\text{infinity}) = 0$ .

2. Consider a d-dimensional system of spins, which can point up ( $s_i=+1$ ) or down ( $s_i=-1$ ). Only nearest neighbors interact („Ising-Model“). We would like to write a Monte Carlo program with which we can determine the statistical properties of such a system.
- a. How many interactions need to be calculated after a single spin flip in d=1,2,3 dimensions?

- d=1: 2 nearest neighbor interactions  
 d=2: 4 nearest neighbor interactions  
 d=3: 6 nearest neighbor interactions



- b. Write down which steps need to be implemented to simulate the Ising model.

Generate starting configuration

|: Flip a single spin

Calculate interactions with nearest neighbors

Energy lower? → Accept the move

Energy higher? → Accept with probability  $\exp(-\beta\Delta E)$

[ Draw random number  $0 < r < 1$  :

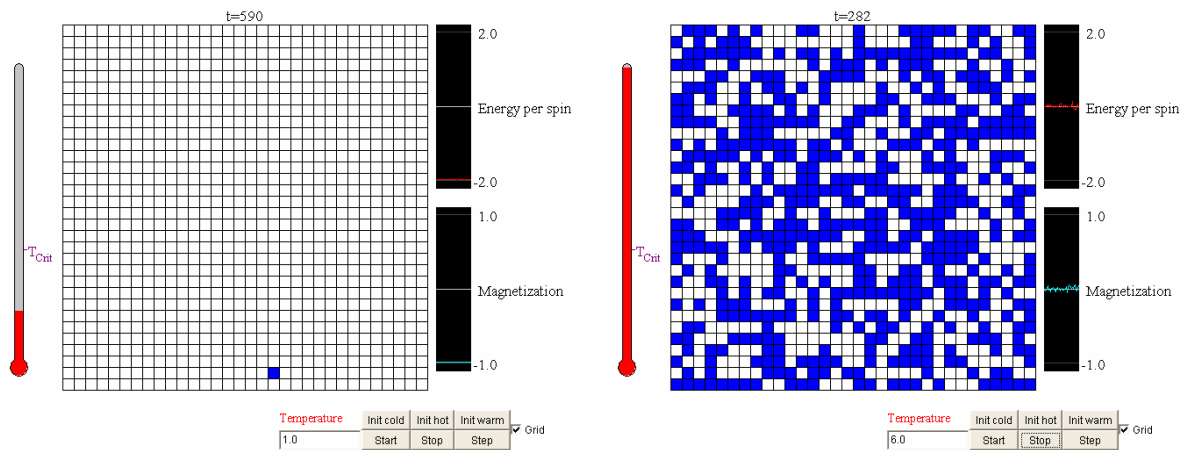
$r < \exp(-1/kT \Delta E)$  → accept spin flip

else → reject spin flip ] :|

c. Which configurations would you expect at high and at low temperatures. Distinguish between  $d=1$  and  $d=2,3$ .

$d=1$ : No phase separation at  $T > 0$

$d=2, d=3$ :

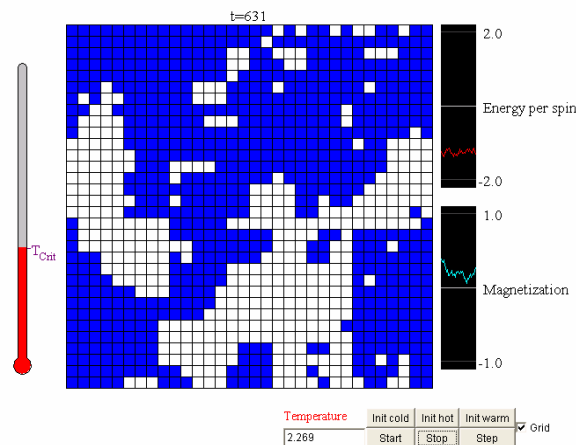


d. If you have access to a computer:

Verify part c for  $d=2$ :

(<http://bartok.ucsc.edu/peter/java/ising/keep/ising.html>)

What happens at  $T=2.629$ ?



Picture credits: [oscar.cacr.caltech.edu/Hrothgar/Ising/Ising1.JPG](http://oscar.cacr.caltech.edu/Hrothgar/Ising/Ising1.JPG)