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)

$\Delta E>0$: $W_{ij}=\exp(-\beta\Delta E)$, $W_{ji}=1$ → $W_{ij}/W_{ji}=\exp(-\beta\Delta E)$ 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: $\tanh(x)=(e^x-e^{-x})/(e^x+e^{-x})$.)

$x=\beta\Delta E/2$

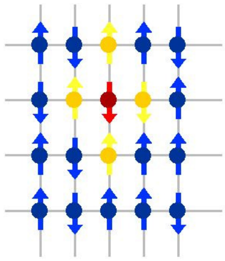
$1-(e^x-e^{-x})/(e^x+e^{-x})$ / $(1-(e^{-x}-e^x)/(e^{-x}+e^x)) = e^{-2x}=\exp(-\beta\Delta E)$ q.e.d.

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

No overlap: Wij=1,
Overlap: Wij=exp(-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

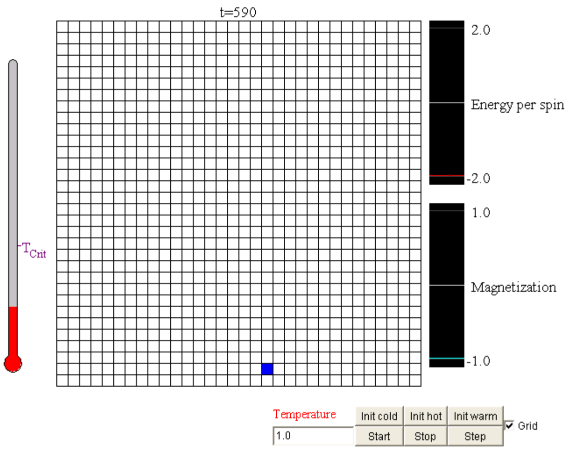
   b. Write down which steps need to be implemented to simulate the Ising model.

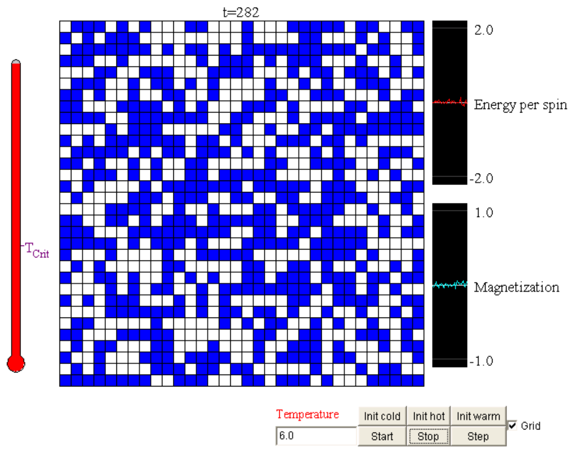
   Generate starting configuration

   |: Flip a single spin
   Calculate interactions with nearest neighbors
   Energy lower? → Accept the move
   Energy higher? → Accept with probability $\exp(-\beta\Delta E)$

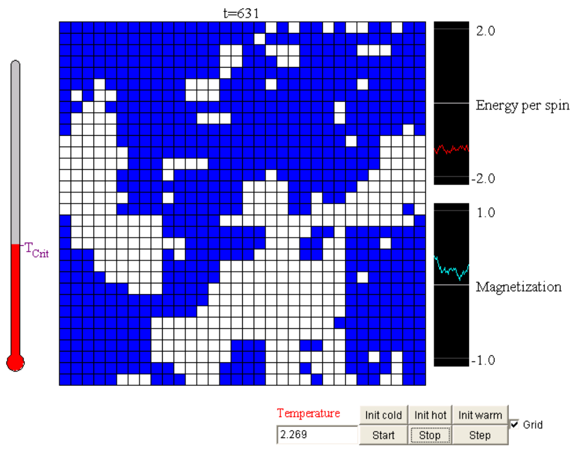
   [Draw random number 0<r<1 :
   r < exp(-1/kT DE) → accept spin flip
   else → reject spin flip] :|

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?



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