Simulations in Statistical Physics

Course for MSc physics students

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Homework 1

3D diffusion-limited aggregation. Responsible: György Vida

Write a computer simulation of the three-dimensional diffusion-limited aggregation model on a simple cubic lattice. Use noise reduction as well. Introduce your own measure of anisotropy and investigate its dependence on the noise reduction and also on the size of the aggregate. How large systems should we choose to see the anisotropy?

`Description:  Ea12.pdf`

Homework 2

Event-driven molecular dynamics. Responsible: Miklós Werner

Investigate the properties of the two-dimensional gas of rigid homogeneous disks with mass m and radius R! The disks can also rotate. The energy is conserved in each collision and there is also an angular momentum exchange.
Write an event-driven simulation! Use periodic boundary conditions! Let the density of disks be the half of the maximal density! Preparate the system in a nonequilibrium state, where the initial angular momentum of the disks is zero. Wait until the system thermalizes and then perform measurements!

- Calculate the average energies for the rotational and translational degrees of freedom. Check equipartition theorem!
- Estimate the distribution of ω, v_x and v_y. Did you get the theoretically predicted result?
- Estimate the distribution of $v = \sqrt{v_x^2 + v_y^2}$ Did you get the two-dimensional Maxwell-Boltzmann distribution?

Homework 3

Epidemic model on BA graph Responsible: László Ujfalusi

Generate a Barabási-Albert graph with parameter m=2. Investigate the following epidemic model on this network:
There are three kinds of nodes: susceptible (**S**), infected (**I**), recovered (**R**). In every time step an infected node infects its susceptible neighbours with probability β, infected sites can recover with probability μ. A recovered site cannot become infected again, and they do not infect any susceptible site.
In the beginning every site is susceptible, except one which is infected. Let T be the time when half of the sites are **I** or **R**. Investigate how T depends on β! Does T ever exist? Perform ensemble average over at least 100 realizations. Use system size $N = 1000$, $\mu = 0.1$.
`Description:`
`http://en.wikipedia.org/wiki/Barabási-Albert_model`

Homework 4

Wolff cluster algorithm Responsible: Gábor Mándi

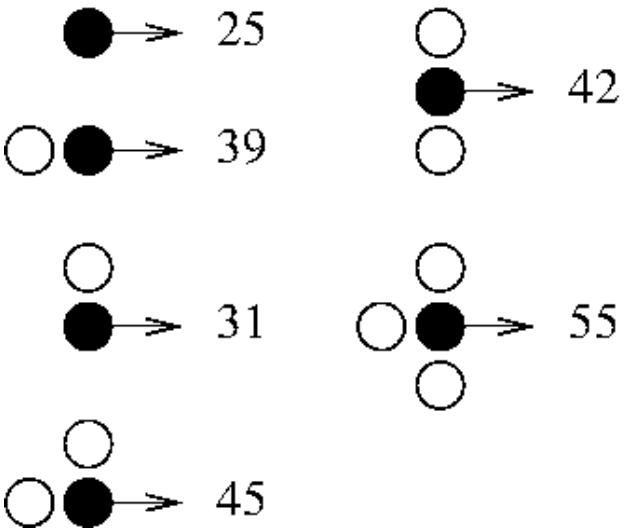
Write a program that uses the Wolff cluster algorithm for the Ising model on the two-dimensional hexagonal lattice!

- Determine the spontaneous magnetization as a function of the temperature and system size.
- Apply finite size scaling to the problem.

Homework 5

Dynamical Monte Carlo simulation Responsible: Balázs Nagyfalusi

Simulate a lattice gas with Kinetic Monte Carlo. Only nearest neighbor interactions are considered. The transition energy barriers ΔE are defined by the following table. Simulate a system of $L = 5$, 10, 20 periodic lattice with particles $N = L^2/4$. Determine the β_c melting temperature. At $\beta = 1.1\beta_c$ measure the diffusion coefficient.



Homework 6

Hawk-dove game Responsible: Marcell Stippinger

Consider the symmetric hawk-dove game on networks, where strategies are Defecting or Cooperating. The game is described by the gain matrix

	D	C
D	0.0	1.6
C	0.2	1.0

In each round, every player plays with all of his/her first neighbours and sums his/her gains of that round. After each round, s/he changes to the most beneficial strategy s/he observed, considering only the gains of him/herself and his/her neighbours in the last round.

Start the game with half of the players playing C, the others D. Examine the evolution of the proportion of C on Barabási-Albert (m=2) and Erdős-Rényi graphs with the same edge density. Consider multiple realizations of the graphs of sizes $n = 2^k$, $(3 \leq k \leq 10)$. Which feature of the graphs may explain the difference in C?

Homework 7

Lattice gas model with random int.s Responsible: Levente Rózsa

Consider an $N \times N$ square lattice with periodic boundary conditions and the following Hamiltonian: $H = -\sum_{\langle ij \rangle} K_{ij}\rho_i\rho_j$. The summation goes over the nearest neighbour pairs. The $K_{ij} = \pm 1$ coefficients are randomized at the start of the simulation, m is the number of particles and $\rho_i = \{0, 1\}$ is the number of atoms. Determine the ground state of the system: for a given set of coupling coefficients, change the positions of the atoms to minimize the energy, but keep the number of atoms constant. For the energy minimization use simulated annealing: introduce the thermodynamical inverse temperature β and use the Metropolis algorithm to determine the probability of moving an atom to an empty lattice point. Start from a higher temperature and decrease it until the system freezes into a local energy minimum. Repeat the simulation to get a better approximation for the minimum value. Do the simulation for two different lattice sizes: N=10, m=50; N=20, m=200.

Calculation of the entropy, free energy, etc.

- Equilibrium statistical physics: From F we can calculate everything
- In simulations F and S cannot be measured directly
- $F = E - TS$ so one of them is enough (E and T are known)
- Solution:
  Calculate the specific heat!

$$C = k_B T^2 \langle (\Delta E)^2 \rangle$$

- The energy fluctuations are measurable
- Since

$$C = T \frac{\partial S}{\partial T}$$

We have

$$S(T) = S(T_0) + \int_{T_0}^{T} \frac{C(T')}{T'} dT'$$

Calculation of the entropy, free energy, etc.

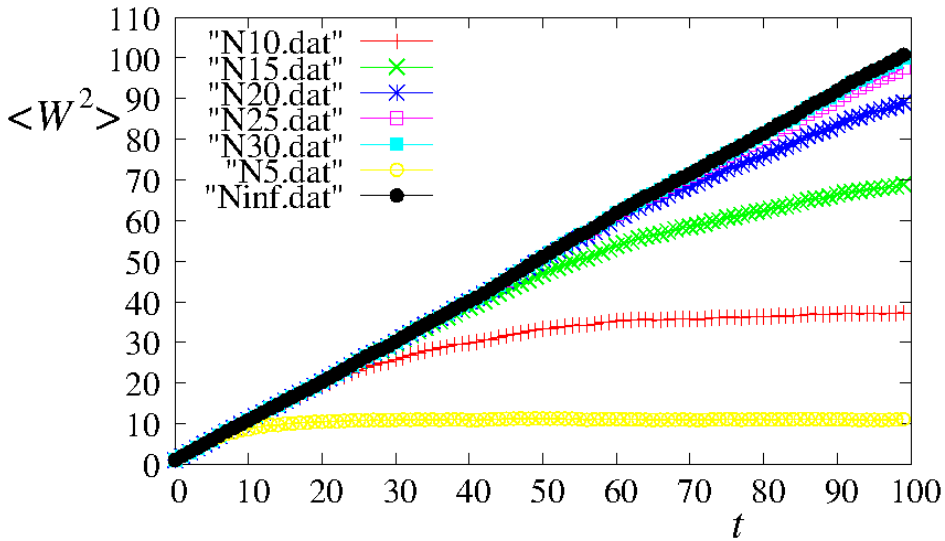
- In many cases derivate of the entropy is needed so $S(T_0)$ is not important in

$$S(T) = S(T_0) + \int_{T_0}^{T} \frac{C(T')}{T'} dT'$$

- From third law of thermodynamics: $S(T = 0) = 0$.

Diffusion

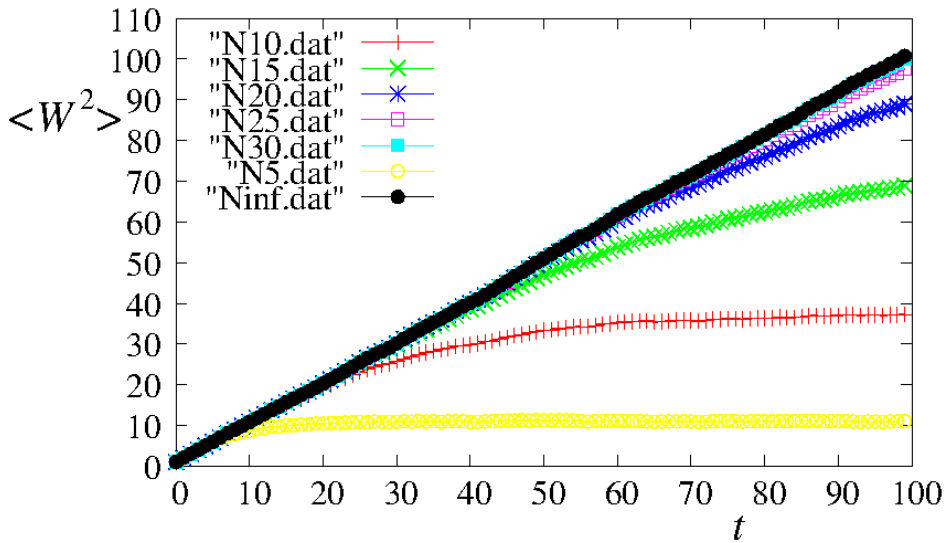
- On normal lattice exactly sovable
- Otherwise e.g. Monte Carlo kinetics. E.g. 1D
  - With probability $1/2 \rightarrow$ go right
  - With probability $1/2 \rightarrow$ go left
  - Be careful with boundary conditions



- Can easily be biased
- Can be simulated on spurious lattices, e.g. Parcolation clusters

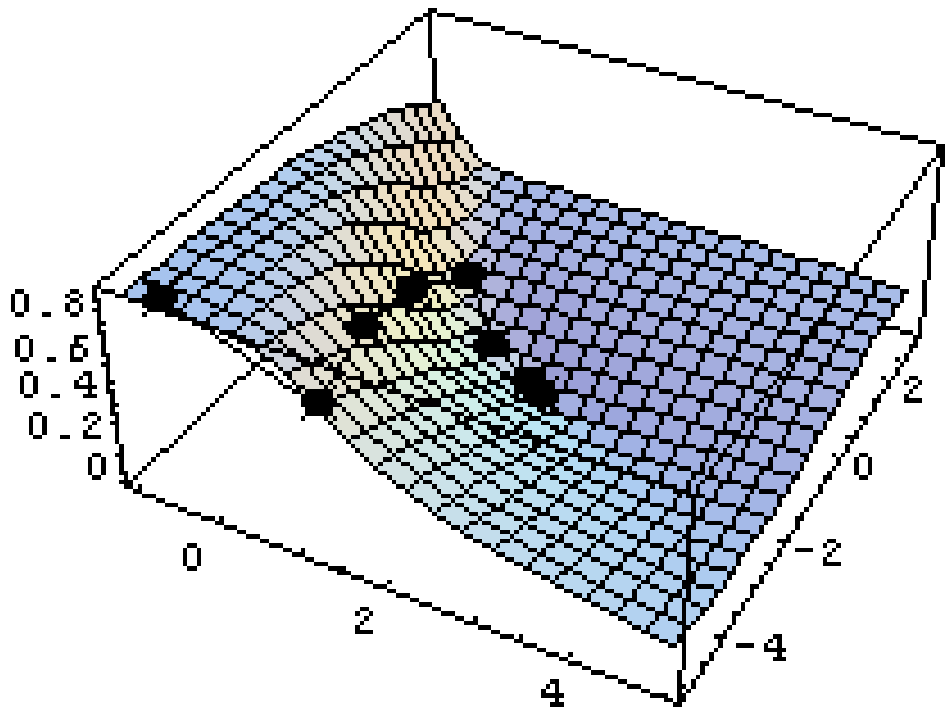
Diffusion

- Solution for diffusion on finite lattice:
- Count steps in both directions
- The net move is $W = n_+ - n_0$
- Use ensemble average
- Plot $\langle W^2 \rangle$ vs. t



Optimization

- General problem of finding the ground state
- Phase-space:
- Arbitrary number of dimensions
- Methods:
  - Steepest Descent
  - Stimulated Annealing
  - Genetic algorithm



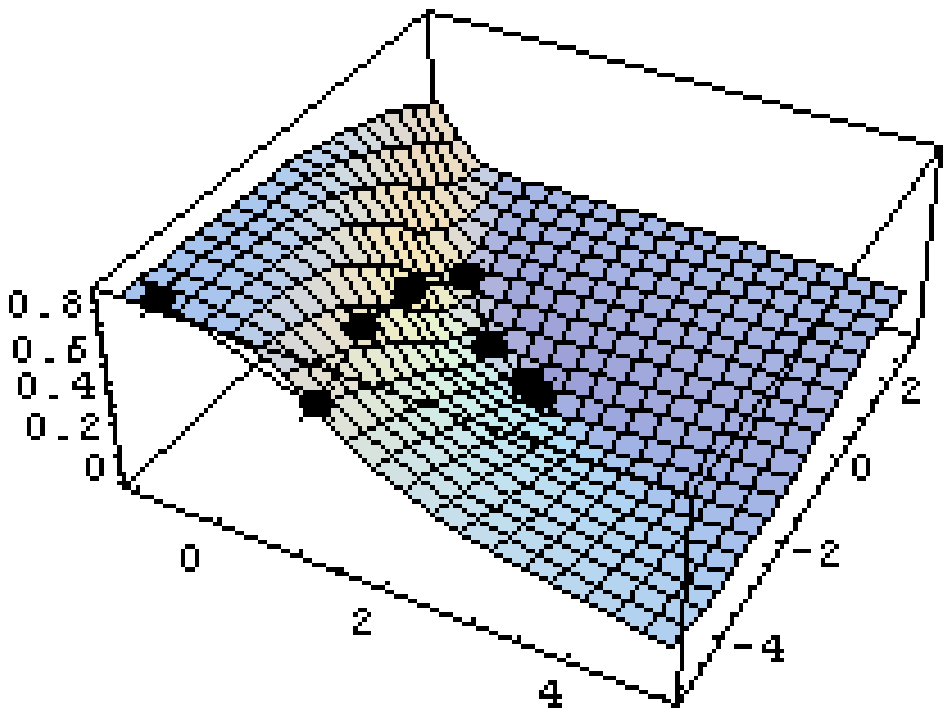
Gradient based optimization

- Given $f(\mathbf{x})$, with $\mathbf{x} = \{x_1, x_2, \ldots x_n\}$
- Gradient $\nabla f(\mathbf{x}) \equiv \mathbf{g}(\mathbf{x}) = \{\partial_1 f, \partial_2 f, \ldots \partial_n f\}$
- Second order partial derivatives: square symmetric matrix called the *Hessian matrix*:

$$\nabla^2 f(\mathbf{x}) \equiv H(\mathbf{x}) \equiv \begin{pmatrix} \partial_1\partial_1 f & \ldots & \partial_1\partial_n f \\ \vdots & \ddots & \vdots \\ \partial_1\partial_n f & \ldots & \partial_n\partial_n f \end{pmatrix}$$

General Gradient Algorithm

1. Test for convergence
2. Compute a search direction
3. Compute a step length
4. Update **x**



Steepest descent algorithm

1. Start from $\mathbf{x}_0$
2. Compute $\mathbf{g}(\mathbf{x}_k) \equiv \nabla f(\mathbf{x}_k)$. If $||\mathbf{g}(\mathbf{x}_k)|| \leq \varepsilon_g$ then stop, otherwise, compute normalized search direction $\mathbf{p}_k = -\mathbf{g}(\mathbf{x}_k)/||\mathbf{g}(\mathbf{x}_k)||$
3. Compute α_k such that $f(\mathbf{x}_k + \alpha \mathbf{p}_k)$ is minimized
4. New point: $\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha \mathbf{p}_k$
5. Test for $|f(\mathbf{x}_{k+1} - f(\mathbf{x}_k))| \leq \varepsilon_a + \varepsilon_r |f(\mathbf{x}_k)|$ and stop if fulfilled in two successive iterations, otherwise go to 2.

Conjugate Gradient Method

1. Start from $\mathbf{x}_0$
2. Compute $\mathbf{g}(\mathbf{x}_k) \equiv \nabla f(\mathbf{x}_k)$. If $||\mathbf{g}(\mathbf{x}_k)|| \leq \varepsilon_g$ then stop, otherwise Go to 5
3. Compute $\mathbf{g}(\mathbf{x}_k) \equiv \nabla f(\mathbf{x}_k)$. If $||\mathbf{g}(\mathbf{x}_k)|| \leq \varepsilon_g$ then stop, otherwise continue
4. Compute the new conjugate gradient direction $\mathbf{p}_k = -\mathbf{g}_k + \beta_k \mathbf{p}_{k-1}$, where

$$\beta = \left(\frac{||\mathbf{g}_k||}{||\mathbf{g}_{k-1}||} \right)^2$$

5. Compute α_k such that $f(\mathbf{x}_k + \alpha \mathbf{p}_k)$ is minimized
6. New point: $\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha \mathbf{p}_k$
7. Test for $|f(\mathbf{x}_{k+1} - f(\mathbf{x}_k))| \leq \varepsilon_a + \varepsilon_r |f(\mathbf{x}_k)|$ and stop if fulfilled in two successive iterations, otherwise go to 3.

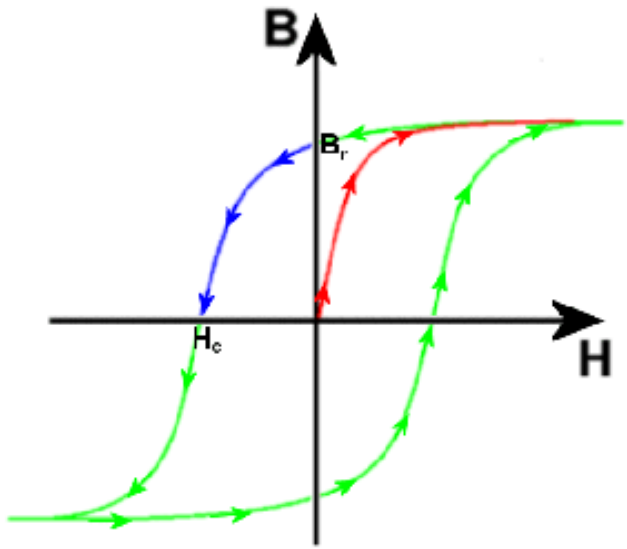
Modified Newton's method

Second order method

1. Start from $\mathbf{x}_0$
2. Compute $\mathbf{g}(\mathbf{x}_k) \equiv \nabla f(\mathbf{x}_k)$. If $||\mathbf{g}(\mathbf{x}_k)|| \leq \varepsilon_g$ then stop, otherwise, continue
3. Compute $H(\mathbf{x}_k) \equiv \nabla^2 f(\mathbf{x}_k)$ and the search direction $\mathbf{p}_k = -H^{-1}\mathbf{g}_k$
4. Compute α_k such that $f(\mathbf{x}_k + \alpha \mathbf{p}_k)$ is minimized
5. New point: $\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha \mathbf{p}_k$
6. Go to 2.

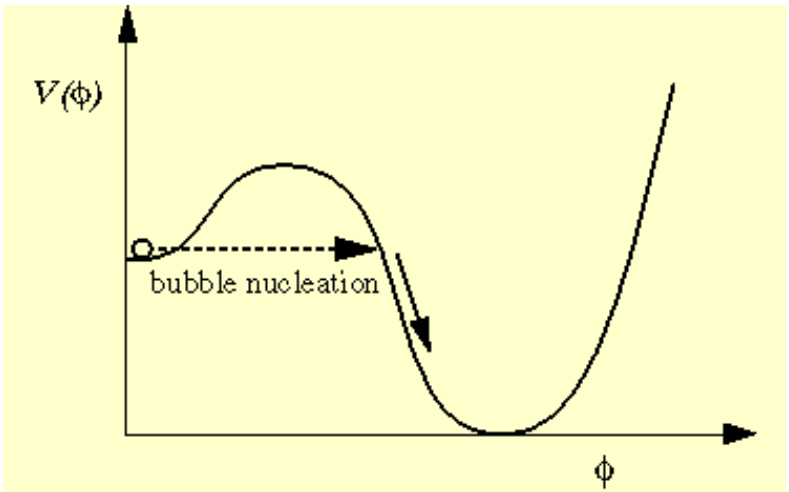
Metastability

- At first order transitions the correlation length remains finite.
- The mechanism of the first order transition is usually nucleation, which is related to metastability.
- Examples can be observed at hysteresis or undercooling, overheating, over-compessing etc.



Nucleation

- There is a competition between the bulk free energy of the droplet and its surface energy
- There is a critical nucleus size above which the transition is very rapid.
- However, such a critical nucleus has to be created by spontaneous fluctuations – which takes (sometimes enormously long) time.

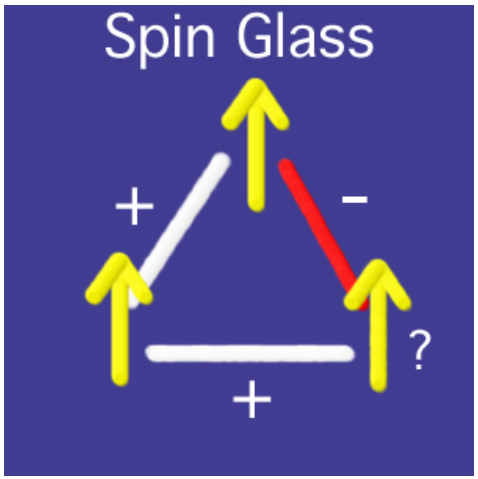


Glassy behavior, frustration

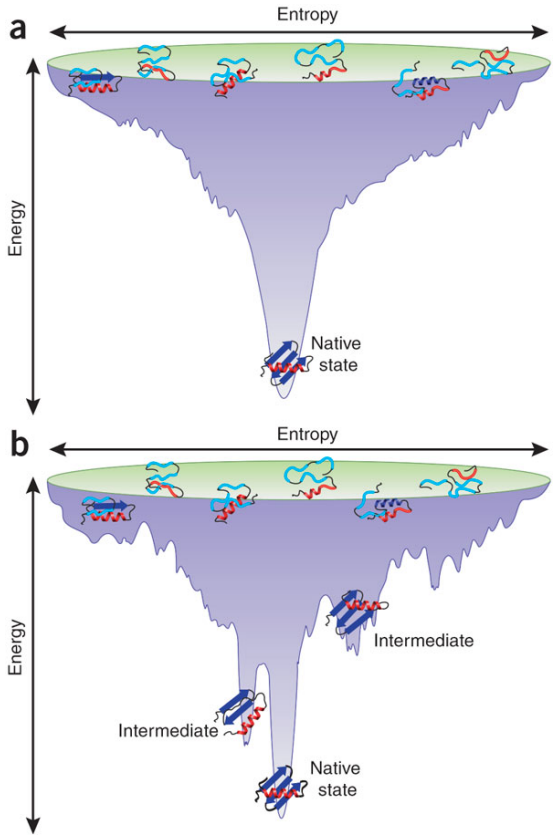
- Model glass: spin-glass:

$$H = -\frac{1}{2}\sum_{\langle i,j\rangle} J_{ij} S_i S_j$$

- where J_{ij} are random quenched variables with 0 mean (e.g. $\pm J$ with probability half)



Rugged energy landscape.



Rugged energy landscape

- Typical example NP-complete problems:
  - Traveling salesman
  - Graph partitioning
  - Spin-glass
- No full optimization is possible (do we need it?)
- Very good minimas can be obtained by optimization
  - Simulated annealing
  - Genetic algorithm

Simulated annealing

- Cool down the system slowly
- Warm up and down if needed, if the system quenched into a local minimum
- One needs a Hamiltonian and an elementary move
- Traveling salesman
  - Path length
  - Exchange two cities in the path
- Use Metropolis simulated annealing. ($T \sim$ alcohol)

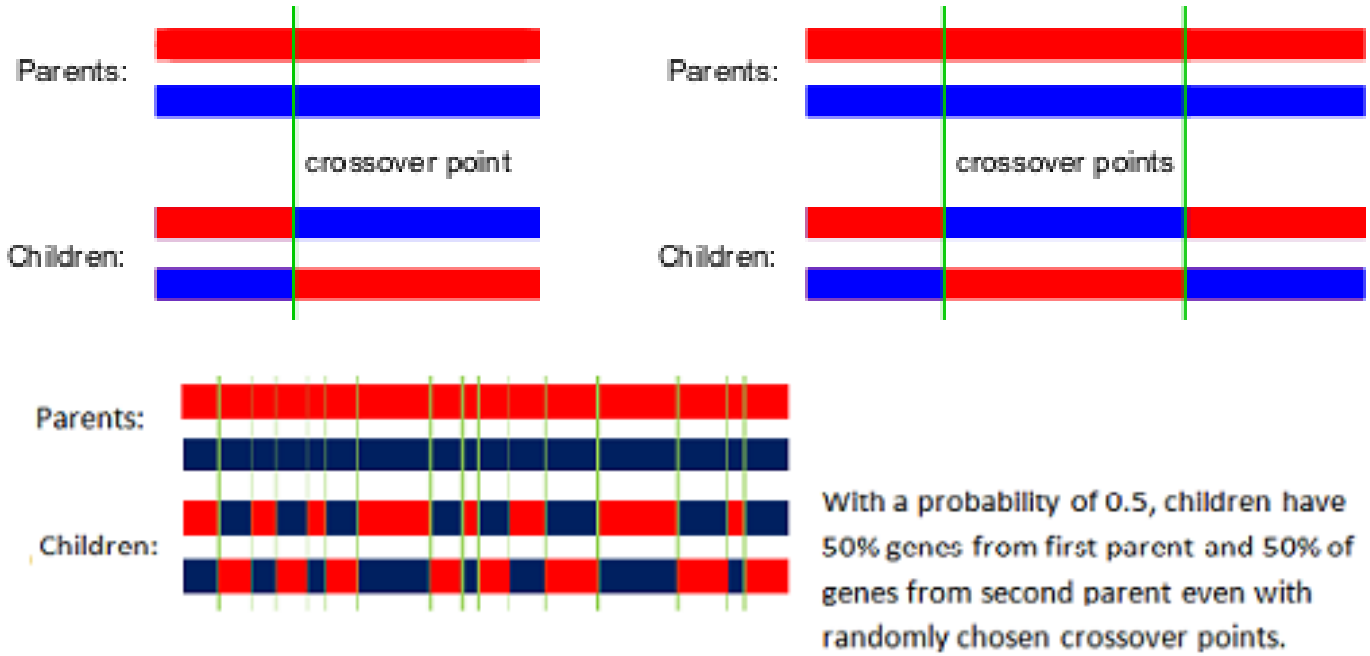
Demo movie

Genetic algorithm

- Learn from nature
- Let the fittest to survive
  - Fitness function, e.g. energy, length, etc.
- Combine different strategies
- State is represented by a vector (genetic code or genotype)
  - Phasespace, city order, neural network parameters, etc.
- Offsprings have two parents with shared genetic code
- Mutations
- Those who are not fit enough die out
  - Keep the number of agents fixed

Genetic algorithm: Reproduction

- Two parents and two children



Genetic algorithm terminology

- Chromosome: Carrier of the genetic representation
- Gene: Smallest units in the chromosome with individual meaning
- Parents: Pair of chromosomes, wich produce offsprings
- Population: Set of chromosomes from which the parents are selected. Its size should be larger than the length of the chromosome
- Selection principle: The way parents are selected (random, elitistic)
- Crossover: Recombination of the genes of the parents by mixing
- Crossover rate: The rate by which crossover takes place ($\sim$90%)
- Mutatation: Random change of genes
- Mutation rate: The rate by which mutation takes place ($\sim$1%)
- Generation: The pool after one sweep.

Genetic algorithm terminology