

Simulations in Statistical Physics

Course for MSc physics students

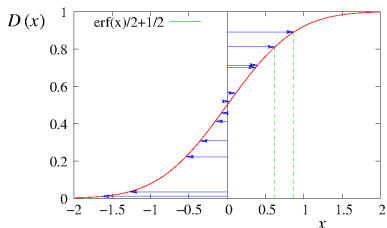
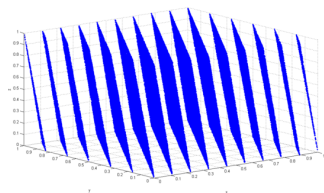
Janos Török

Department of Theoretical Physics

December 18, 2013

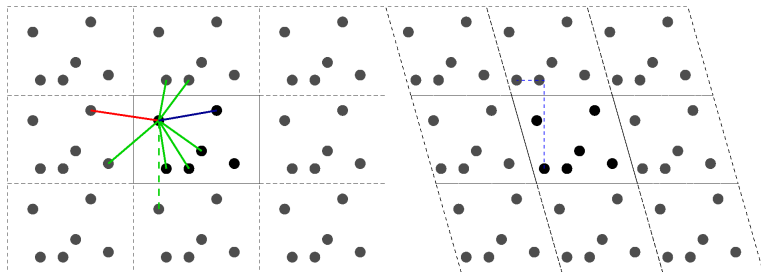
Random numbers

- ▶ Random number generators
- ▶ Problems (e.g. Marsaglia effect)
- ▶ Random numbers with different distributions



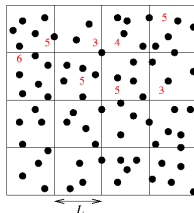
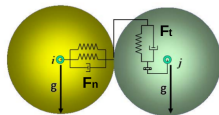
Boundary conditions

- ▶ Periodic boundary conditions
- ▶ Periodic boundary conditions deformed box
- ▶ Distance

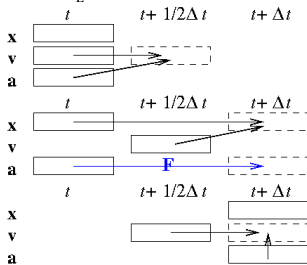


Molecular dynamics

- ▶ Algorithm
- ▶ Applications
- ▶ Forces
 - ▶ Pair
 - ▶ Frictional
- ▶ Find pairs
 - ▶ Bucketing algorithm
 - ▶ k-space solution
- ▶ Integration
 - ▶ Euler method
 - ▶ Runge-Kutta method
 - ▶ Leapfrog method
 - ▶ Verlet method
 - ▶ Multiscale
- ▶ Temperature
 - ▶ Nosé-Hoover thermostat

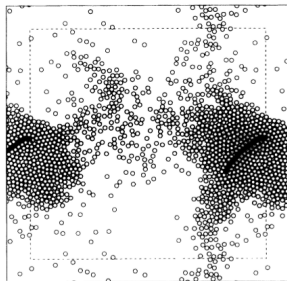
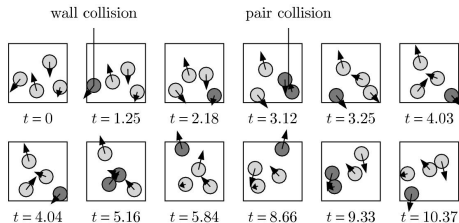


`b[0,0]={1,7,9,147,8};`
`b[0,1]={12,8,99};`



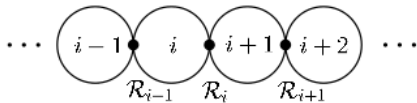
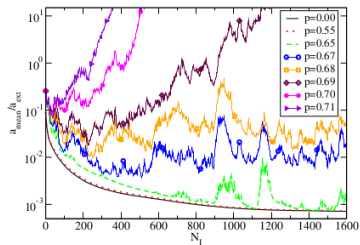
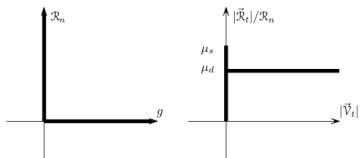
Event driven algorithm

- ▶ Algorithm
- ▶ Application
- ▶ Inelastic collapse



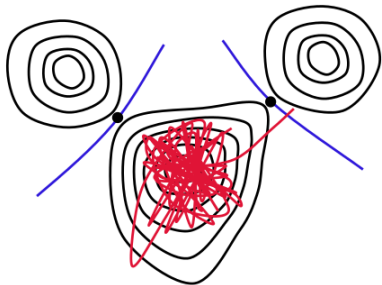
Contact dynamics

- ▶ Algorithm
- ▶ Application
- ▶ Iterative solver
- ▶ Elasticity



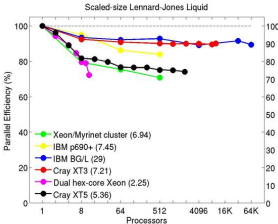
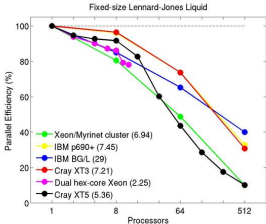
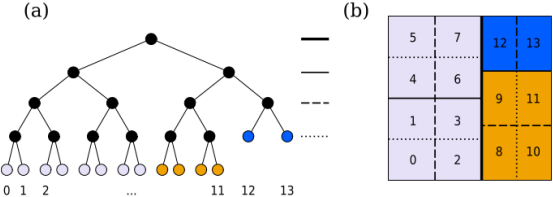
Kinetic Monte Carlo

- ▶ Algorithm
- ▶ Application



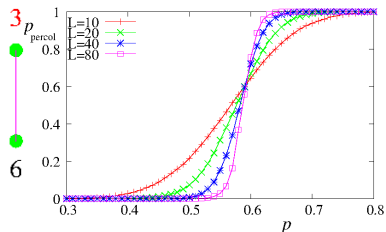
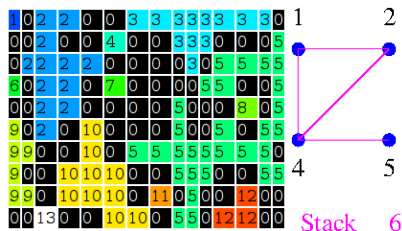
Parallelization

- ▶ How, why?
- ▶ Algorithm



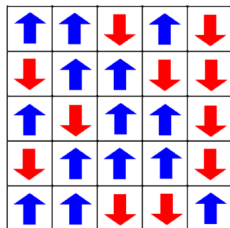
Percolation

- ▶ Definition
- ▶ Hoshen-Kopelman Algorithm
- ▶ Percolation on networks (graphs)
- ▶ Algorithm percolation on networks (graphs)
- ▶ Determine p_c



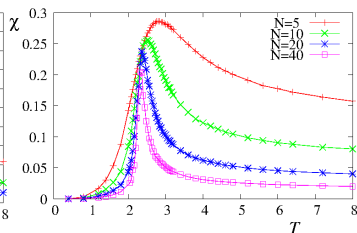
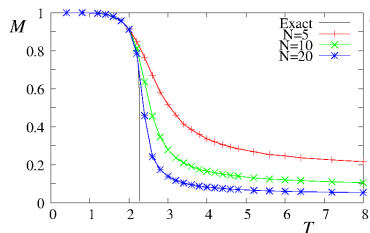
Ising-model

- ▶ Definition
- ▶ Importance sampling
- ▶ Characteristic time
- ▶ Metropolis algorithm



Finite size scaling

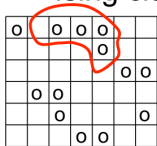
- ▶ Finite size effects
- ▶ Algorithm
- ▶ Fit



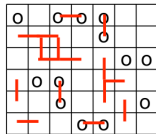
Ising model

- ▶ Multi-spin
- ▶ Cluster algorithm
 - ▶ Swendsen-Wang algorithm
 - ▶ Wolff algorithm
- ▶ Kawasaki dynamics

Ising cluster

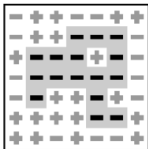


Ising configuration

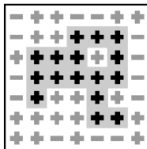


Ising „droplets”

A Wolff droplet (gray)
before flipping



a

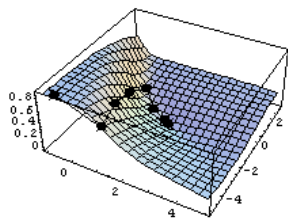


b

The new configuration
The droplet contour is
still shown, though the
bonds are eliminated
after flipping

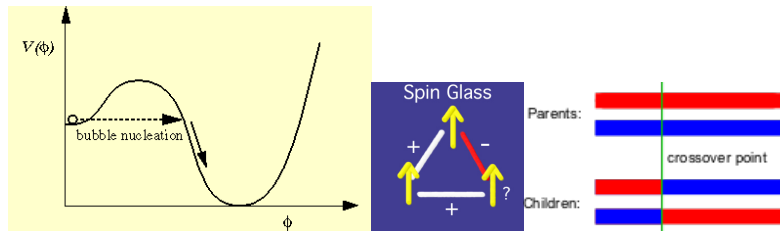
Optimization

- ▶ Gradient based optimization
- ▶ Steepest descent algorithm
- ▶ Conjugate Gradient Method
- ▶ Modified Newton's method



Glassy behavior

- ▶ Metastability
- ▶ Nucleation
- ▶ Frustration
- ▶ Simulated annealing
- ▶ Genetic algorithm

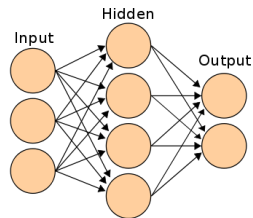
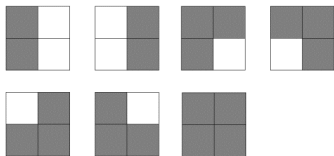
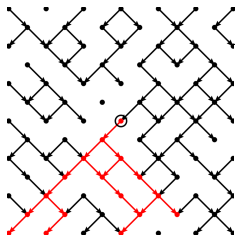


Growth models

- ▶ DLA
 - ▶ Algorithm
 - ▶ Optimization
 - ▶ Noise reduction
 - ▶ Anisotropy
- ▶ Dielectric breakdown model
- ▶ Eden model
- ▶ Ballistic deposition
- ▶ KPZ-equation

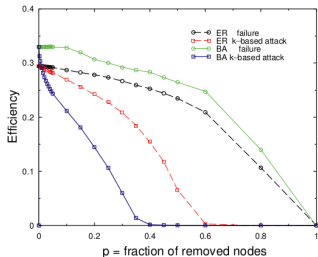
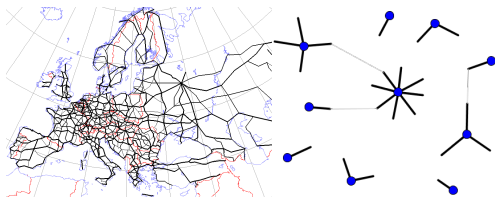
Discrete models

- ▶ Directed percolation
 - ▶ Exponents
- ▶ Numerical renormalization group
 - ▶ Fix points
- ▶ Neural networks



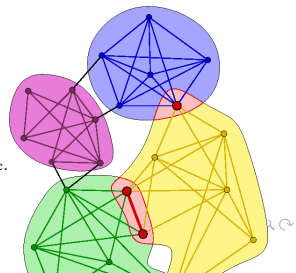
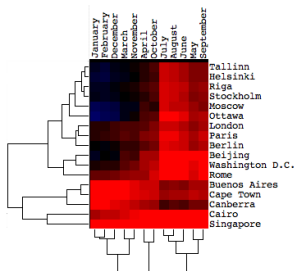
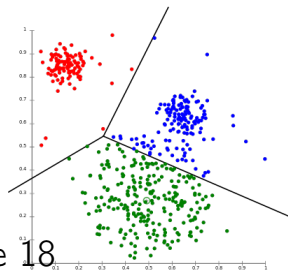
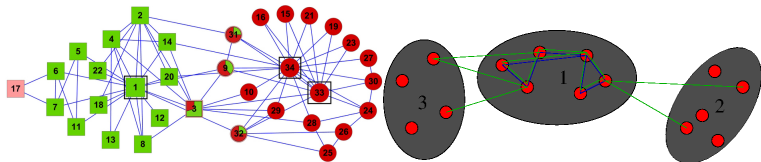
Complex networks

- ▶ Random Networks
 - ▶ Erdős-Rényi graph
 - ▶ Configurations model
 - ▶ Barabási-Albert model
- ▶ Percolation and attack on random networks



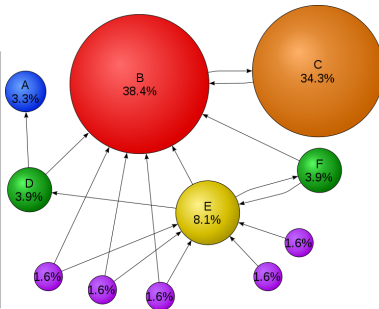
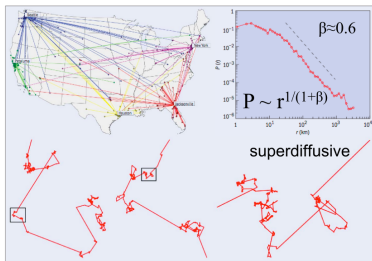
Clustering

- ▶ Definitions, local, global
 - ▶ Modularity
 - ▶ k-means clustering
 - ▶ Hierarchical clustering
 - ▶ LFK method
 - ▶ Clique percolation



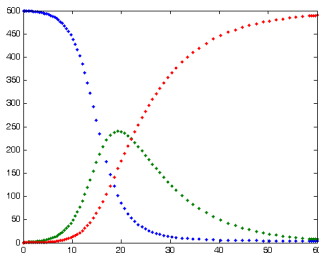
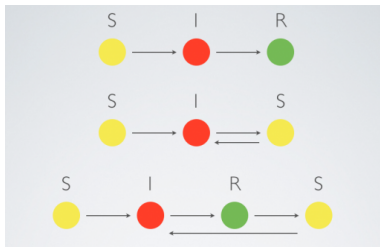
Random walk on networks

- ▶ Random walk master eq.
- ▶ Solution on uncorrelated network
- ▶ Page rank



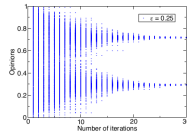
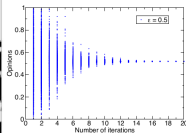
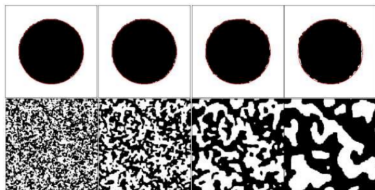
Disease spreading

- ▶ SIR model
- ▶ Algorithm
- ▶ Bit coding



Opinion models

- ▶ Ising $T = 0$
- ▶ Voter model
- ▶ Bounded confidence model
- ▶ Hegselmann-Krause model



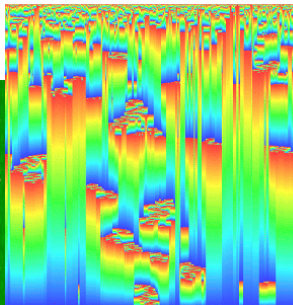
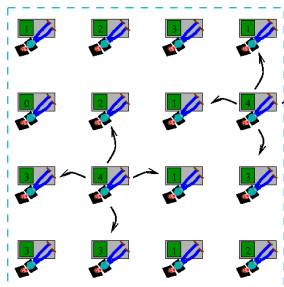
Game models

- ▶ Rock-paper-scissors
- ▶ Prisoner's dilemma
- ▶ Chicken, hawk-dove game

	Cooperate	Defect
Cooperate	Reward	S, T
Defect	T, S	Punish

Self-Organized Criticality

- ▶ Definition
- ▶ Bak-Tang-Wiesenfeld model
- ▶ Forest fire
- ▶ Bak-Sneppen model of evolution



Traffic models

- ▶ Nagel–Schreckenberg model
- ▶ Emergence of traffic jams
- ▶ Asymmetric simple exclusion process

