Simulations in Statistical Physics Lecture 12

János Kertész

BME Department of Theoretical Physics

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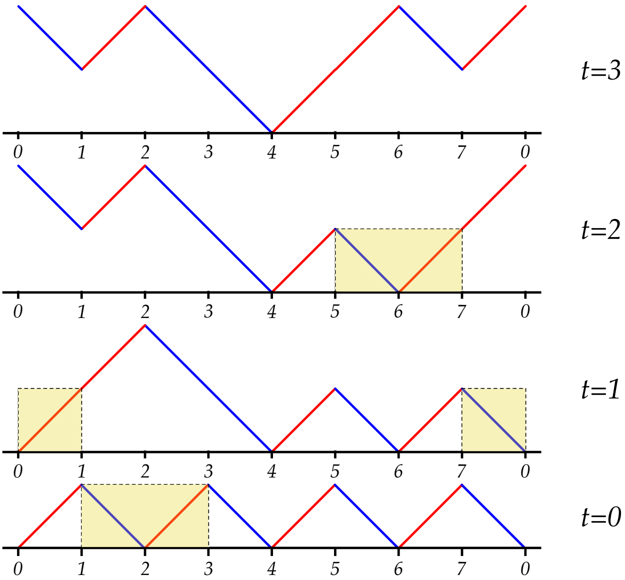
Homework

- C, C++, Fortran
- Documentation (.pdf, .doc):
  - Algorithm and implementation details
  - Interpretation of the results
- Source code (with an abundance of comments)
- Send **at least 1 week prior to the examination** to racze@phy.bme.hu.
- Tasks available at: `http://tinyurl.com/36j2qah`

Single Step on Solid Model



Single Step on Solid

$h_i(t)$: surface height at time t above point i, $i = 0, 1, \ldots, N-1$

$w(N,t)$: surface width

$$w(N,t) \equiv \sqrt{\frac{1}{N-1}\sum_{i=0}^{N-1}\left(h_i(t) - \overline{h}(N,t)\right)^2}$$

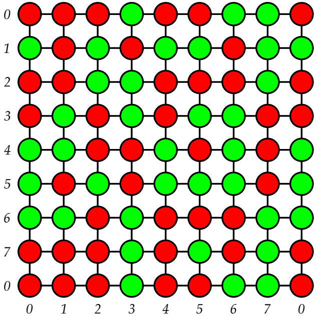
$$\overline{h}(N,t) \equiv \frac{1}{N}\sum_{i=0}^{N-1} h_i(t) = ?$$

Scaling: crossover time $t_x \propto N^z$, and

$$w(N,t) = L^\alpha f\left(\frac{t}{L^z}\right) \propto \begin{cases} t^\beta & t \ll t_x \\ N^\alpha & t \gg t_x \end{cases}$$

$$\boxed{z, \alpha, \beta = ?}$$

Prisoner's Dilemma on a Square Lattice



	Coop.	Def.
Coop.	(1,1)	(3,0)
Def.	(0,3)	(2,2)

Prisoner's Dilemma on a Square Lattice

1. Random strategies (cooperate with prob. p)
2. At each timestep, choose random neighbors, they play the game
3. For the next step, each player chooses the strategy of the neighbor (including himself) who gained the most up to time t.
4. Go to the second step.

What is the asymptotic proportion of cooperative players as a function of p?

Maximal Spanning Tree

- Download the 2006-2009 daily historical prices for the 30 stocks included in the Dow Jones Industrial Average (`http://finance.yahoo.com/q/cp?s=^DJI+Components`)
- For each of the 4 years, calculate the correlation matrix of the daily returns ($r_t^{(i)} \equiv \log p_{t+1}^{(i)} - \log p_t^{(i)}$)
- These matrices can be regarded as the adjacency matrix of a fully connected weighted graph.
- Calculate the *maximal spanning tree* (the spanning tree for which the sum of the edge weights is maximal) for each matrix. (`http://en.wikipedia.org/wiki/Prim's_algorithm`)
- Compare the spanning trees gained by this method.

Ising Spin Glass

- $\mathcal{H} = -\sum_{\langle i,j \rangle} J_{ij} \cdot s_i s_j$, $s_i = \pm 1$, $\mathbb{P}(J_{ij} = \pm J) = 1/2$
- Determine the ground state energy (per site) on a square lattice of size 10×10 and 20×20 using a genetic algorithm. (http://newton.phy.bme.hu/~kertesz/Ea8.pdf)
- Use periodic boundary conditions.

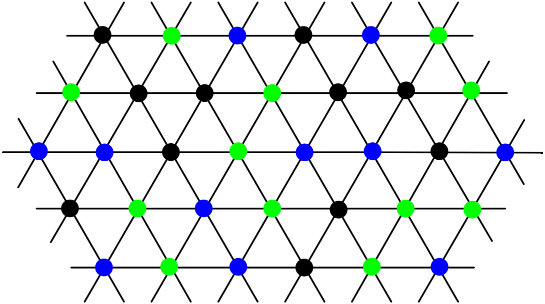
2D Hard Disk Fluid

- Write an event-driven molecular dynamics simulation for a hard disk fluid.
- Use periodic boundary conditions.
- Let the density be $\rho = 0.5 \cdot \rho_{\text{max}}$.
- Determine the pair-correlation function

$$g(r) \equiv \frac{\mathbb{E}\left[\#\left\{i : |\mathbf{r}_i| \in [r, r+\delta r) \mid \exists \text{ mol. at the origin}\right\}\right]}{2\pi r \delta r \cdot \rho}$$

3-state Potts Model on a Triangular Lattice

$$\mathcal{H} \equiv -K \sum_{\langle i,j \rangle} \delta_{S(i),S(j)}, \;\; S(i) \in [0,1,2]$$



- $\boxed{T_c = ?}$
- Apply finite size scaling to the problem.

Betweenness Centrality

- Betweenness centrality: c_i is the proportion of shortest paths leading through node i:

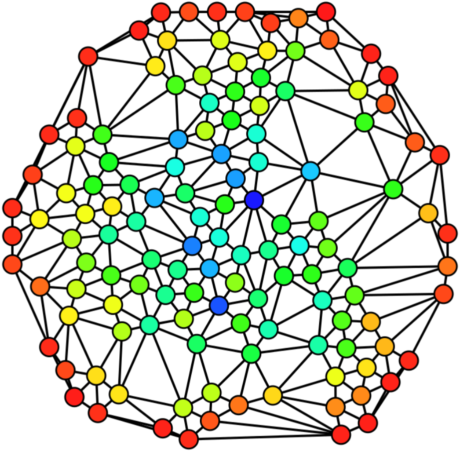
$$c_i \equiv \frac{\#\left\{k, l \neq i, k < l : i \in p_{k \to l}\right\}}{\left(N-1\right)\left(N-2\right)/2}, \quad \text{with}$$

$$p_{k \to l} \equiv \text{the shortest path from } k \text{ to } l$$

- Generate a 1000-point Barabási–Albert graph (let $k = 2$).
- Determine how c_i depends on the degree of node i:

$$\overline{c}\left(d\right) \equiv \frac{1}{\#\left\{i : d_i = d\right\}} \sum_{i : d_i = d} c_i$$

Betweenness Centrality



http://en.wikipedia.org/wiki/Centrality

http://www.cs.ucc.ie/~rb4/resources/Brandes.pdf

The Kardar–Parisi–Zhang Model

A surface-growth model that incorporates rejection of particles from the surface (void formation).

$$\partial_t h(\mathbf{x}, t) = F + \nu \nabla^2 h + \lambda (\nabla h)^2 + \eta(\mathbf{x}, t)$$

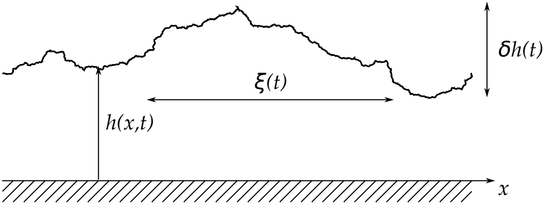
$h(\mathbf{x}, t)$: The height of a layer above a d-dimensional surface ($\mathbb{R}^{d+1} \to \mathbb{R}$)

$\eta(\mathbf{x}, t)$: Gaussian white noise

$$\langle \eta(\mathbf{x}, t) \rangle = 0$$
$$\langle \eta(\mathbf{x}, t)\, \eta(\mathbf{x}', t') \rangle = A \delta^d(\mathbf{x} - \mathbf{x}')\, \delta(t - t')$$

$$h(\mathbf{x}, t) \to h(\mathbf{x}, t) - F \cdot t$$

KPZ model – Scaling Behavior



$$\xi(t) \propto t^{1/z}$$

$$\delta h(t) \propto t^{\zeta/z} \propto \xi(t)^{\zeta}$$

$$\delta h(L,t) \equiv \sqrt{L^{-d}\int_{L^d} \mathrm{d}^d x \left[h(\mathbf{x},t) - \overline{h}(L,t)\right]^2} = L^{\zeta} f\left(L/\xi(t)\right)$$

$$f(x) \begin{cases} = \text{const.} & L < \xi(t) \\ \propto x^{-\zeta} & L > \xi(t) \end{cases}$$

KPZ model – Scaling Behavior

- The linear case ($\lambda = 0$) is exatly solvable by Fourier trf. ($d = 1$: $z = 2$, $\zeta = 1/2$; $d = 2$: $z = 2$, $\delta h^2 \propto \log \xi$)
- Nonlinear case ($\lambda \neq 0$): the coupling constant $g \equiv F\lambda^2/\nu^3$ determines the behavior.

Space Discretization, 1D

$x_i = i\Delta x,\ h_i = h(x_i)$

$$\frac{\partial h}{\partial x}(x_i) = \frac{h_{i+1} - h_{i-1}}{2\Delta x} + O\left(\Delta x^2\right)$$

$$\left[\frac{\partial h}{\partial x}(x_i)\right]^2 = \frac{\left(h_{i+1} - h_{i-1}\right)^2}{4\Delta x^2} + O\left(\Delta x^2\right)$$

$$\frac{\partial^2 h}{\partial x^2}(x_i) = \frac{h_{i+1} - 2h_i + h_{i-1}}{\Delta x^2} + O\left(\Delta x^2\right)$$

$\Downarrow$

$$\frac{\mathrm{d}h_i}{\mathrm{d}t} = \frac{1}{\Delta x^2}\left[\nu\left(h_{i+1} - 2h_i + h_{i-1}\right) + \frac{\lambda}{4}\left(h_{i+1} - h_{i-1}\right)^2\right] + \text{noise.}$$

Remark: For the KPZ equation, $\exists$ an intrinsic instability, even in the deterministic part.

Space Discretization of the Noise, 1D

$$\eta_i(t) = \frac{1}{\Delta x} \int_{x_i - \Delta x/2}^{x_i + \Delta x/2} \eta(x, t) \, \mathrm{d}x$$

with this definition,

$$\langle \eta_i(t) \rangle = 0$$

$$\langle \eta_i(t) \eta_j(t') \rangle = \frac{A}{\Delta x} \delta_{ij} \delta(t - t')$$

Time Discretization

Euler scheme: $H_i(t_{n+1}) = H_i(t_n) + \Delta t \cdot \tilde{\partial}_t H_i(t_n)$

$$\Delta H_i = \frac{\Delta t}{\Delta x^2}\Big\{\nu\left[H_{i+1}(t_n) - 2H_i(t_n) + H_{i-1}(t_n)\right] + \frac{\lambda}{4}\left[H_{i+1}(t_n) - H_{i-1}(t_n)\right]^2\Big\} + \sqrt{\frac{A\Delta t}{\Delta x}}\mathcal{N}(0,1)$$

Euler scheme stability: $\Delta t < \text{const.}\,(\Delta x)^z$