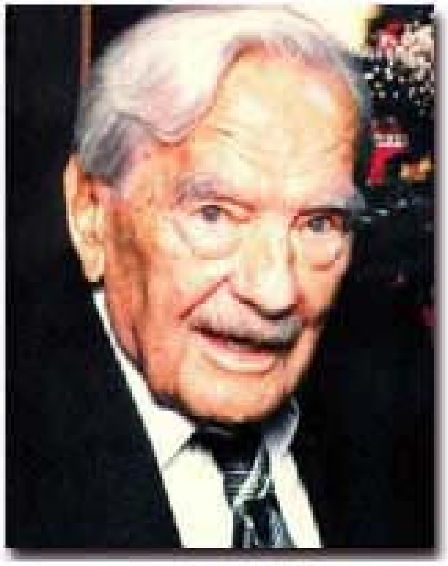
Monte Carlo Methods



Nicholas Constantine Metropolis

Stanislaw Ulam

Books about Monte Carlo

- M.H. Kalos and P.A. Whitlock: „Monte Carlo Methods“ (Wiley-VCH, Berlin, 2008)
- J.M. Hamersley and D.C. Handscomb: „Monte Carlo Methods“ (Wiley & Sons, N.Y., 1964)
- K. Binder and D. Heermann: „Monte Carlo Simulations in Statistical Physics“ (Springer, Berlin, 1992)
- R.Y. Rubinstein: „Simulation and the Monte Carlo Method“ (Wiley & Sons, N.Y., 1981)

Monte Carlo Method (MC)

Simulates an experimental measuring process with sampling and averaging.

Big advantage:

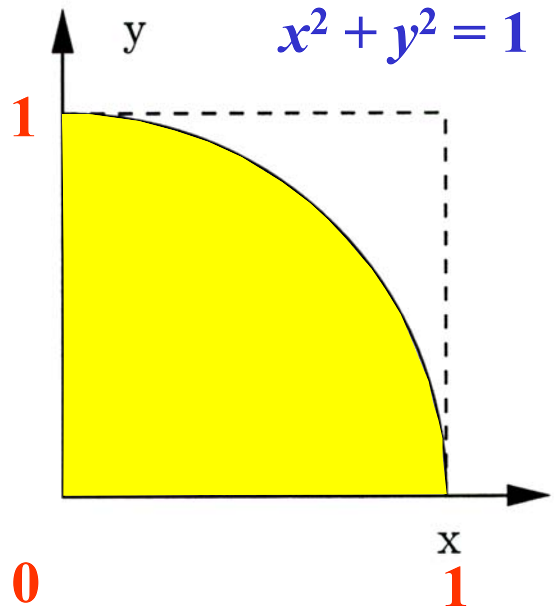
Systematic improvement by increasing the number of samples *N*.

Error goes like: $\boxed{\Delta \propto \frac{1}{\sqrt{N}}}$

Applications of Monte Carlo

- **Statistical partition functions, i.e. averages at constant temperature**
- **High dimensional integrals**

Calculation of π



$$\pi = 4\int_0^1 \sqrt{1-x^2}\,dx$$

Choose N pairs

(x_i, y_i), $i = 1,\ldots,N$

of random numbers

$x_i, y_i \in \{0,1\}$

Calculation of π

$$c = 0$$

$$\text{if} \quad y_i^2 < 1 - x_i^2 \Rightarrow c = c + 1$$

***c* is number of points that fall inside circle.**

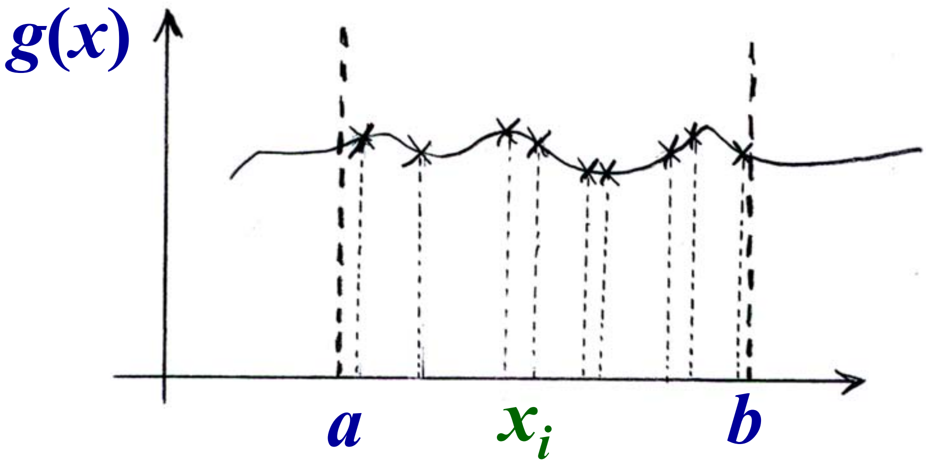
$$\boxed{\textbf{area} \propto c/N}$$

$$\boxed{\pi(N) = 4\frac{c}{N}}$$

applet

$$\boxed{\Delta = \pi - \pi(N) \propto \frac{1}{\sqrt{N}}}$$

Calculation of integrals



$$\int_a^b g(x)dx \approx (b-a)\left[\frac{1}{N}\sum_{i=1}^{N} g(x_i)\right]$$

Calculation of integrals

random numbers $x_i \in [a,b]$

homogeneously distributed:

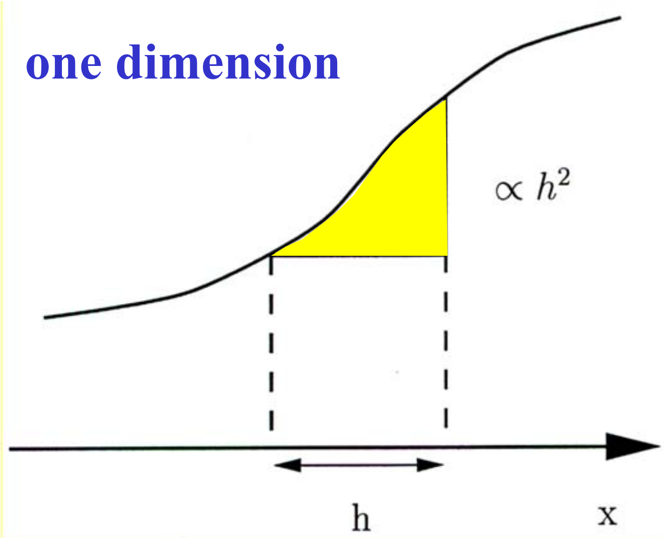
„simple sampling“

Good if $g(x)$ smooth.

Error of integration

conventional method:

choose N equidistant points $\Rightarrow$ distance $\boxed{h = \frac{b-a}{N}}$



$$\boxed{\text{area} \propto h^2 \propto \frac{1}{N^2} \propto \frac{1}{T^2}}$$

where T is the computer time.

error:

$$\boxed{\Delta \propto (N\ \text{area})^2 \propto T^{-2}}$$

Error in d dimensions

in d dimensions: $\boxed{h \propto \frac{1}{L} \;,\; T \propto N = L^d \quad \Rightarrow \quad h \propto T^{-\frac{1}{d}}}$

error with conventional method:

$$\boxed{\Delta \propto \left(Nhh^d\right)^2 \propto T^2 h^{2(d+1)} \propto T^{-\frac{2}{d}}}$$

error with Monte Carlo: $\boxed{\Delta \propto \frac{1}{\sqrt{N}} \propto T^{-\frac{1}{2}}}$

$\Rightarrow$ Monte Carlo better for $d > 4$

High dimensional integral

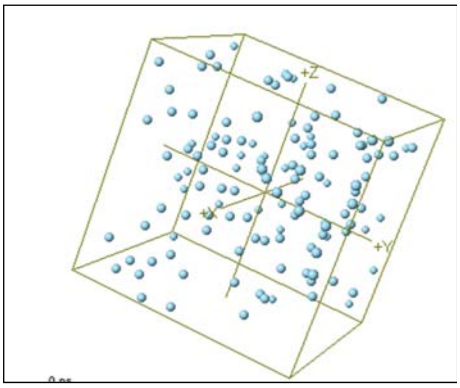
Consider n hard spheres of radius R in a 3d box.

Phase space is 3n dimensional: (x_i, y_i, z_i), $i = 1,\ldots,n$.

$$r_{ij} = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2}$$

with hard sphere constraint

$$\sqrt{(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2} > 2R$$



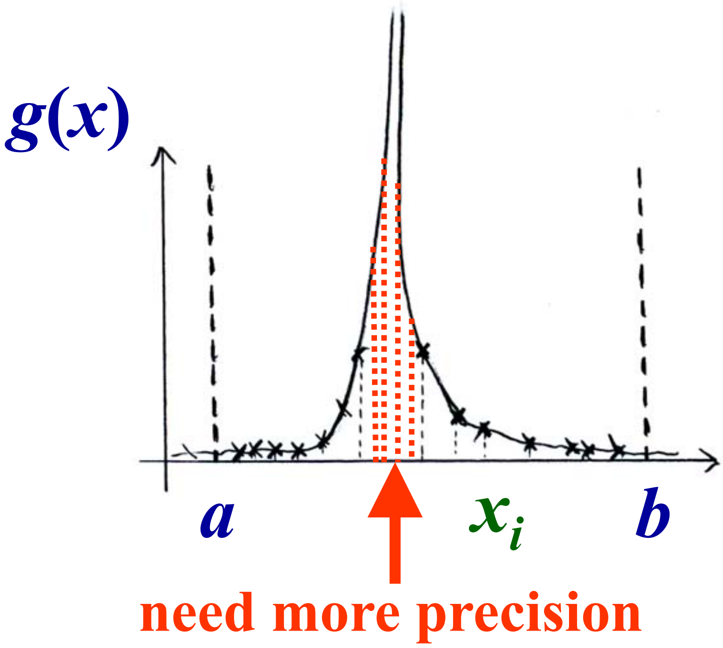
Calculate average distance:

$$< r_{ij} > = \frac{1}{Z} \int \frac{2}{n(n-1)} \sum_{i<j} r_{ij} dx_1, \ldots, dx_n dy_1, \ldots, dy_n dz_1, \ldots, dz_n$$

MC strategy

- **Choose particle position.**
- **If the excluded volume condition is not fulfilled then reject.**
- **Once the n particles are placed, calculate the average of r_{ij} over all pairs (i,j).**

Not smooth integrals



Calculation of integrals

$$\boxed{\int_a^b g(x)dx = \int_a^b \frac{g(x)}{p(x)} p(x)dx \approx (b-a)\frac{1}{N}\sum_{i=1}^{N}\frac{g(x_i)}{p(x_i)}}$$

if x_i randomly distributed according to $p(x)$.

Good convergence when function $\frac{g(x)}{p(x)}$ smooth.

„importance sampling“

Canonical Monte Carlo

$E(X)$ = energy of configuration X

Probability for system to be in X is given by Boltzmann factor:

$$p_{eq}(X) = \frac{1}{Z_T} e^{-\frac{E(X)}{kT}}$$

Z_T is the partition function:

$$Z_T = \sum_X e^{-\frac{E(X)}{kT}}$$

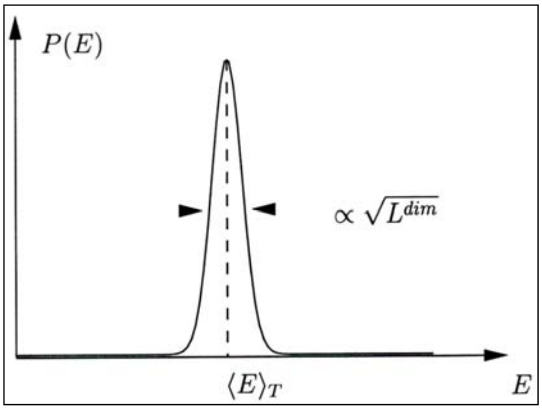
$$\sum_X p_{eq}(X) = 1$$

Problem of sampling

$$< Q(T) >= \sum_X Q(X) p_{eq}(X)$$

thermal average

The distribution of energy E around the average $< E >_T$ gets sharper with increasing size.



Choosing configurations equally distributed over energy would be very ineffective.

M(RT)^2 algorithm

N.C. Metropolis, A.W. Rosenbluth,
M.N. Rosenbluth, A.H. Teller and E. Teller (1953)

importance sampling through a Markov chain:

$$X_1 \rightarrow X_2 \rightarrow \ldots..$$

where the probability for a configuration is $p_{eq}(X)$

Markov chain: X_t only depends on $X_{t\text{-}1}$

Properties of Markov chain

Start in configuration X and propose a new configuration Y with probability $T(X \rightarrow Y)$.

1. Ergodicity: One must be able to reach any configuration Y after a finite number of steps.
2. Normalization: $$\boxed{\sum_Y T(X \rightarrow Y) = 1}$$
3. Reversibility: $$\boxed{T(X \rightarrow Y) = T(Y \rightarrow X)}$$

Transition probability

The proposed configuration Y will be accepted with probability $A(X \to Y)$.

Total probability of a Markov chain is:

$$W(X \to Y) = T(X \to Y) \cdot A(X \to Y)$$

Master equation:

$$\boxed{\frac{dp(X,t)}{dt} = \sum_Y p(Y)W(Y \to X) - \sum_Y p(X)W(X \to Y)}$$

Properties of $W(X \to Y)$

- **Ergodicity:** $$\boxed{\forall X, Y : W(X \to Y) > 0}$$
- **Normality:** $$\boxed{\sum_Y W(X \to Y) = 1}$$
- **Homogeneity:** $$\boxed{\sum_Y p_{st}(Y)\; W(Y \to X) = p_{st}(X)}$$

Canonical Monte Carlo

$E(X)$ = energy of configuration X

Probability for system to be in X is given by

Boltzmann factor: $$\boxed{p_{eq}(X) = \frac{1}{Z_T} e^{-\frac{E(X)}{kT}}}$$

Z_T is the partition function:

$$\boxed{Z_T = \sum_X e^{-\frac{E(X)}{kT}}} \qquad \boxed{\sum_X p_{eq}(X) = 1}$$

M(RT)^2 algorithm

importance sampling through a Markov chain:

$$X_1 \to X_2 \to \ldots..$$

where the probability for a configuration is $p_{eq}(X)$

Markov chain: X_t only depends on X_{t-1}

The proposed configuration Y will be

accepted with probability $A(X \to Y)$.

Total probability of a Markov chain is:

$$W(X \to Y) = T(X \to Y) \cdot A(X \to Y)$$

Detailed balance

$$\boxed{\frac{dp(X,t)}{dt} = \sum_Y p(Y)\, W(Y \to X) - \sum_Y p(X)\, W(X \to Y)}$$

In stationary state one should have equilibrium distribution (Boltzmann)

$$\boxed{\frac{dp_{st}(X,t)}{dt} = 0 \quad , \quad \boxed{p_{st}(X) = p_{eq}(X)}}$$

$$\boxed{\Rightarrow \sum_Y p_{eq}(Y)\, W(Y \to X) = \sum_Y p_{eq}(X)\, W(X \to Y)}$$

sufficient condition for detailed balance:

$$\boxed{p_{eq}(Y)\, W(Y \to X) = p_{eq}(X)\, W(X \to Y)}$$

Metropolis (M(RT)²)

$$\boxed{A(X \to Y) = \min\left(1, \frac{p_{eq}(Y)}{p_{eq}(X)}\right)}$$

Boltzmann: $\boxed{p_{eq}(X) = \frac{1}{Z_T} e^{-\frac{E(X)}{kT}}}$

$$\boxed{A(X \to Y) = \min(1, e^{-\frac{E(Y)-E(X)}{kT}}) = \min(1, e^{-\frac{\Delta E}{kT}})}$$

If energy decreases always accept

If energy increases accept with probability $e^{-\frac{\Delta E}{kT}}$.

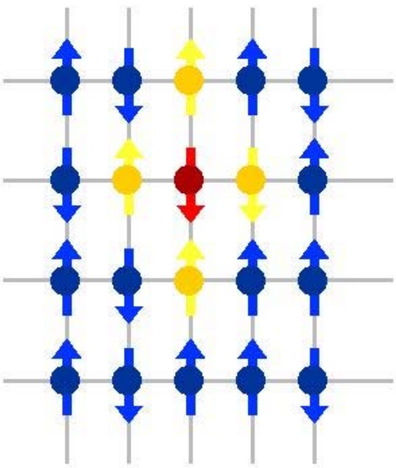
Glauber dynamics

Roy C. Glauber (1963)
(Nobel prize 2005)

$$A(X \rightarrow Y) = \frac{e^{-\frac{\Delta E}{kT}}}{1 + e^{-\frac{\Delta E}{kT}}}$$

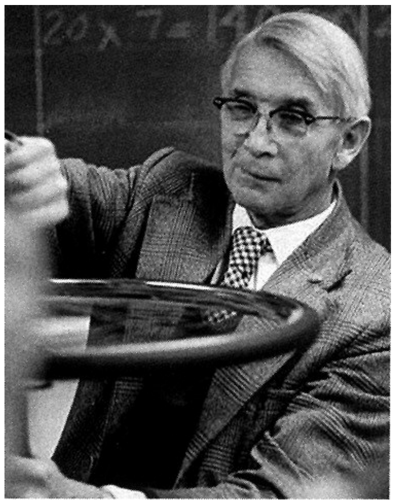
also fulfills detailed balance

The Ising Model



Spins on a lattice

(1924)



Ernst Ising
(1900-1998)

- Magnetic Systems
- Opinion models
- Binary mixtures

The Ising Model

Binary variables:

$$\sigma_i = \pm 1, \qquad i = 1, \ldots, N$$

on a graph of *N* sites

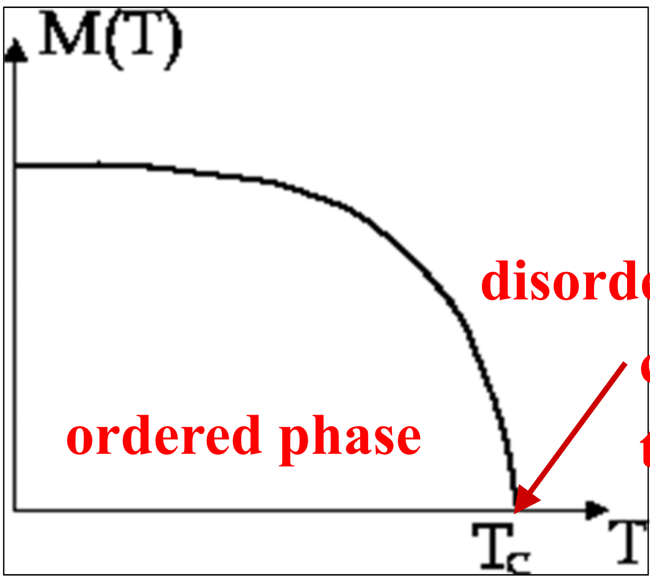
interacting via the Hamiltonian:

$$\mathcal{H} = E = -J \sum_{i,j:nn}^{N} \sigma_i \sigma_j - H \sum_{i=1}^{N} \sigma_i$$

Order parameter

spontaneous magnetization:

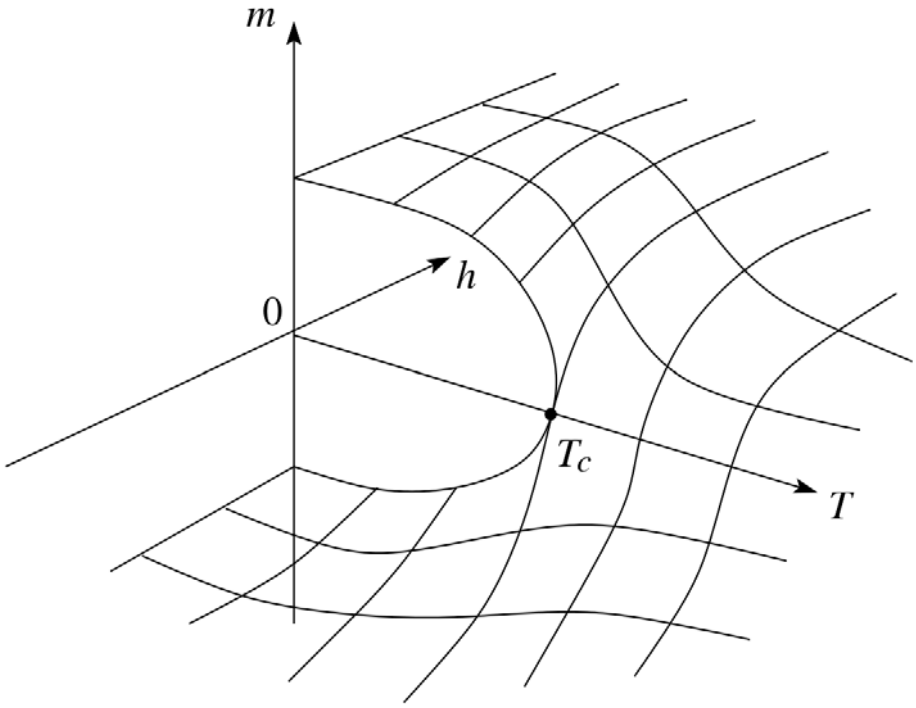
$$M(T) = \lim_{H \to 0} \left\langle \frac{1}{N} \sum_{i=1}^{N} \sigma_i \right\rangle$$



$$\boxed{M \propto (T - T_c)^{\beta}}$$

$$\beta = 1/8 \quad (2d)$$
$$\beta \approx 0.326 \; (3d)$$

Phase diagram



Response functions

susceptibility:

$$\boxed{\chi(T) = \left.\frac{\partial M}{\partial H}\right|_{T,H=0} \propto \left|T - T_c\right|^{-\gamma}}$$

specific heat:

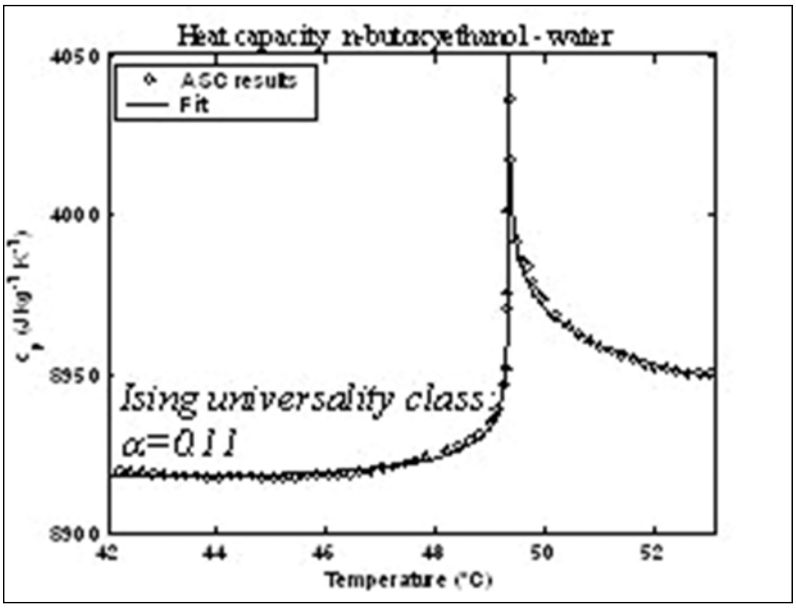
$$\boxed{C_v(T) = \left.\frac{\partial E}{\partial T}\right|_{V,H} \propto \left|T - T_c\right|^{-\alpha}}$$

both diverge at T_c

Specific heat

$$C_v(T) \propto |T - T_c|^{-\alpha}$$

$\alpha = 0$ (2d)
$\alpha \approx 0.11$ (3d)

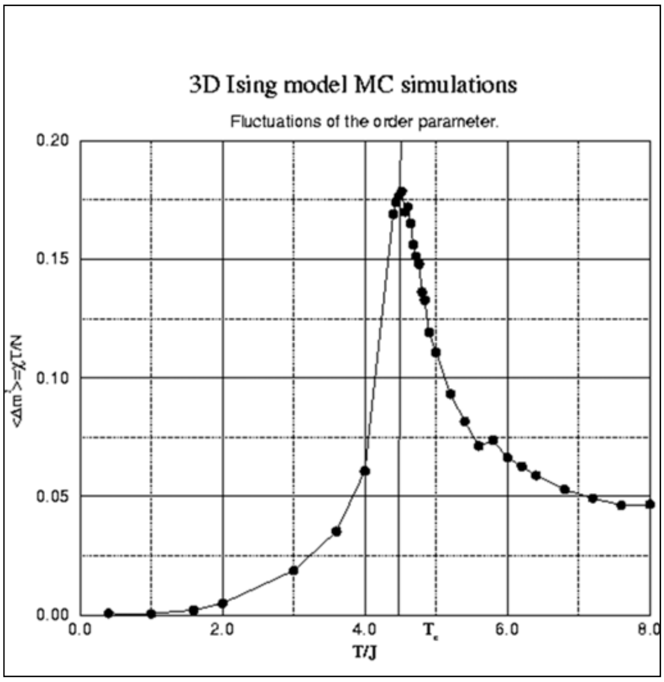


comparing with experimental data for binary mixture

Susceptibility

$$\chi(T) \propto |T - T_c|^{-\gamma}$$

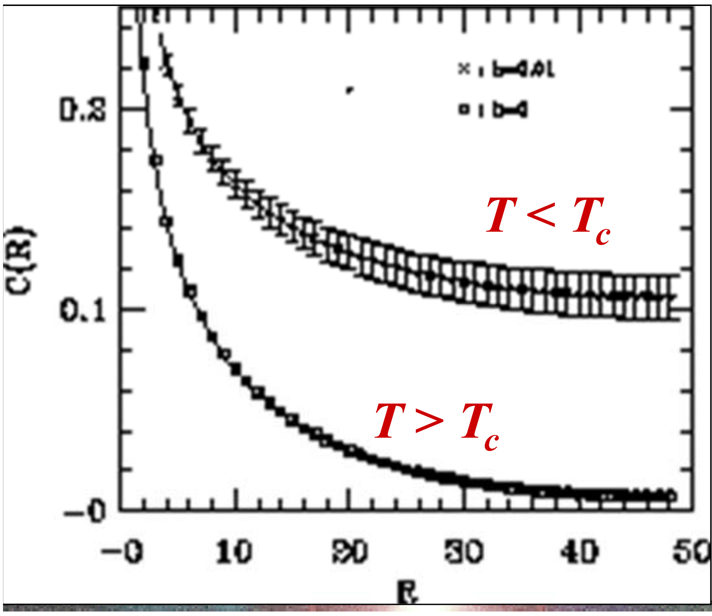
$\gamma = 7/4$ (2d)
$\gamma \approx 1.24$ (3d)



numerical data from a finite system

Correlation length

correlation function: $C(R) = \langle \sigma(0)\sigma(R) \rangle$



For $T \neq T_c$ and for large R:

$$C(R) \propto M^2 + a e^{-\frac{R}{\xi}}$$

where ξ is the correlation length.

Correlation length

The correlation length diverges at T_c as:

$$\xi \propto |T - T_c|^{-\nu}$$

with a critical exponent ν.

$$\nu = 1 \quad \text{(2d)}$$
$$\nu \approx 0.63 \quad \text{(3d)}$$

At T_c we have for large R:

$$C(R) \propto R^{2-d-\eta}$$

with

$$\eta = 1/4 \quad \text{(2d)}$$
$$\eta \approx 0.05 \quad \text{(3d)}$$

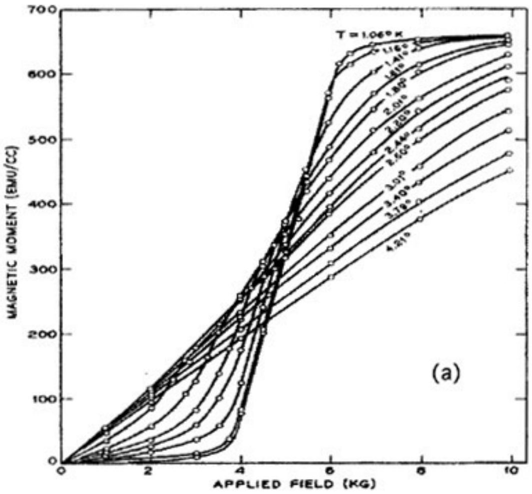
Magnetic exponent

at T_c

$$\boxed{M \propto H^{1/\delta}}$$

$\delta = 15$ **(2d)**

$\delta \approx 4.79$ **(3d)**



DyAlG in field along [111]
above and below Néel temperature

Critical exponents

	d=2	d=3	d=4	
α	0	0.11008(1)	0	2 − d / (d − Δϵ)
β	1/8	0.326419(3)	1/2	Δσ / (d − Δϵ)
γ	7/4	1.237075(10)	1	(d − 2Δσ) / (d − Δϵ)
δ	15	4.78984(1)	3	(d − Δσ) / Δσ
η	1/4	0.036298(2)	0	2Δσ − d + 2
ν	1	0.629971(4)	1/2	1 / (d − Δϵ)
ω	2	0.82966(9)	0	Δϵ′ − d

Exponent relations

Exponents are related through:

$$\boxed{\begin{array}{c}\alpha + 2\beta + \gamma = 2 \\ 2-\alpha = d\nu \\ (2-\eta)\nu = \gamma\end{array}}$$

scaling

hyperscaling

so that only two exponents are independent.

H.E.Stanley, „Introduction to Phase Transitions and Critical Phenomena“ (Clarendon, Oxford, 1971)

Exact solutions

1 dimension:

$$\boxed{Z_N = 2\cosh(\beta J)^N \left[1+\tanh(\beta J)^N\right]}$$

$$\boxed{F(T,H) = -\beta^{-1}\ln\left(2\cosh(\beta J)\right)}$$

Lars Onsager 1944

square lattice:

$$\boxed{\ln Z_T(T,H=0) = \ln\left(2\cosh(2\beta J)\right) + \frac{1}{2\pi}\int_0^{\pi} \ln\frac{1}{2}\left(1+\sqrt{1-\kappa^2\sin^2\phi}\right)d\phi}$$

$$\boxed{\kappa = 2\sinh\left(2\beta J\right)/\cosh^2\left(2\beta J\right)}$$

$$\boxed{\beta = \frac{1}{k_B T}}$$

Metropolis (M(RT)²)

$$\boxed{A(X \to Y) = \min\left(1, \frac{p_{eq}(Y)}{p_{eq}(X)}\right)}$$

Boltzmann: $p_{eq}(X) = \dfrac{1}{Z_T} e^{-\frac{E(X)}{kT}}$

$$A(X \to Y) = \min(1, e^{-\frac{E(Y)-E(X)}{kT}}) = \min(1, e^{-\frac{\Delta E}{kT}})$$

If energy decreases always accept

If energy increases accept with probability $e^{-\frac{\Delta E}{kT}}$.

MC of the Ising Model

$E = -J \sum_{i,j:nn}^{N} \sigma_i \sigma_j$

Single flip Metropolis:

new configuration

old configuration

- **Choose one site i (having spin σ_i).**
- **Calculate $\Delta E = E(Y) - E(X) = 2J\sigma_i h_i$.**
- **If $\Delta E < 0$ then flip spin: $\sigma_i \to -\sigma_i$.**
- **If $\Delta E > 0$ flip with probability $\exp(-\Delta E/kT)$.**

where h_i is the local field at site i $\quad \boxed{h_i = \sum_{nn\ of\ i} \sigma_j}$

applet

Binary mixtures
(lattice gas)

Consider two species A and B distributed with given concentrations on the sites of a lattice.

E_{AA} is energy of A-A bond.

E_{BB} is energy of B-B bond.

E_{AB} is energy of A-B bond.

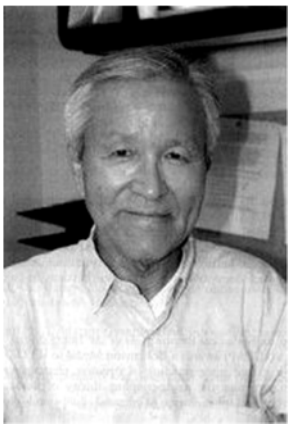
Set $E_{AA} = E_{BB} = 0$ and $E_{AB} = 1$.

Number of each species is constant.

Kawasaki dynamics

- **Choose any A-B bond.**
- **Calculate ΔE for A-B → B-A.**
- **Metropolis: If $\Delta E \leq 0$ flip, else flip with $p = \exp(-\beta\Delta E)$.**
- **Glauber: Flip with probability $p = \exp(-\beta\Delta E)/(1+\exp(-\beta\Delta E))$.**

$$\beta = 1/kT$$



Kyozi Kawasaki

Other Ising-like models

- **Antiferromagnetic models:**

staggered field

$$\mathcal{H} = J \sum_{i,j:nn} \sigma_i \sigma_j + H_s \sum_i (-1)^i \sigma_i$$

- **Ising spin glass:**

random interaction

$$\mathcal{H} = \sum_{i,j:nn} J_{ij} \sigma_i \sigma_j$$

frustration

in x-direction

- **ANNNI model:**

incomensurate phases

with „Lifshitz point“

$$\mathcal{H} = -J_1 \sum_{i,j:nn} \sigma_i \sigma_j + J_2 \sum_{i:nnn} \sigma_i \sigma_{i+2}$$

- **Metamagnets:**

tricritical point

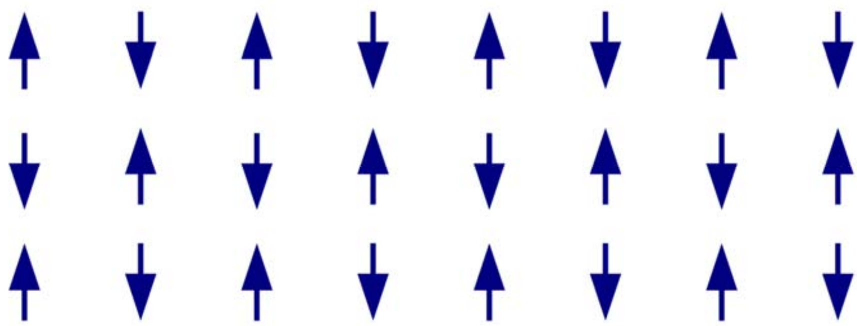
$$\mathcal{H} = J_1 \sum_{i,j:nn} \sigma_i \sigma_j - J_2 \sum_{i,j:nnn} \sigma_i \sigma_j - H \sum_i \sigma_i$$

Antiferromagnetic Ising model

$$\mathcal{H} = J \sum_{i,j:nn} \sigma_i \sigma_j + H_s \sum_i (-1)^i \sigma_i$$

On square lattice phase diagram and critical behavior exactly identical to ferromagnetic case.

staggered field on square lattice



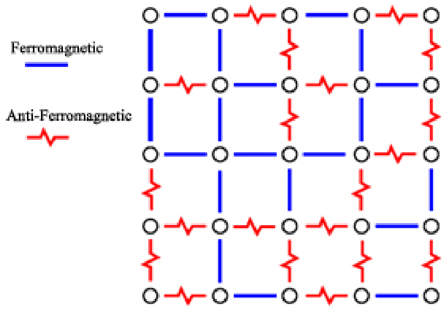
frustration on triangular lattice

On the triangular lattice the critical temperature is zero and the ground state is infinitely degenerate (finite entropy).

Ising spin glass

Edwards Anderson model (1975):

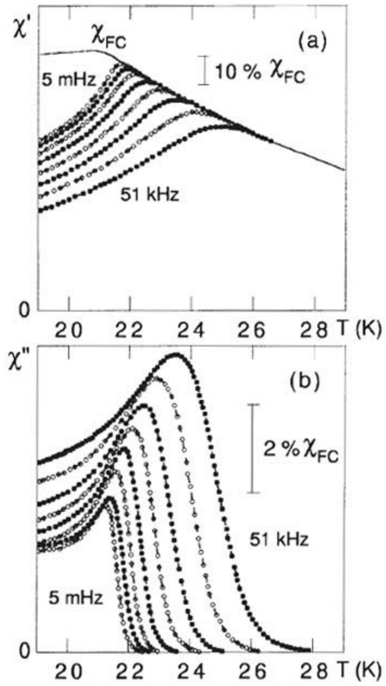
$$\mathcal{H} = \sum_{i,j:nn} J_{ij}\sigma_i\sigma_j \qquad P(J_{ij}) = \frac{1}{2}\left[\delta(J_{ij}+J)+\delta(J_{ij}-J)\right]$$



frustration

freezing of spins

quenched average



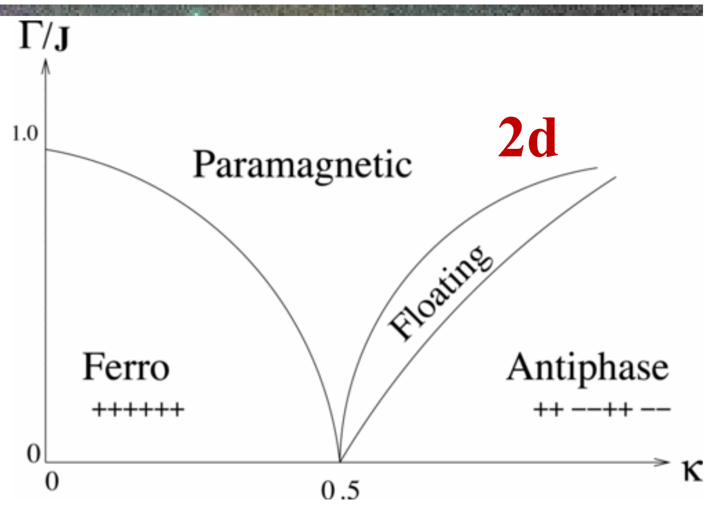
$Fe_{0.5}Mn_{0.5}TiO_3$

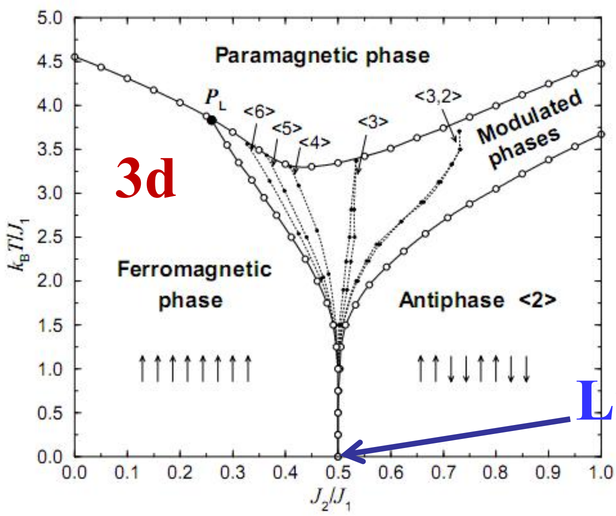
order parameter in spin glass phase ($T<T_c$):

$$q \equiv \frac{1}{N}\sum_{i=1}^{N}\langle\sigma_i\rangle^2 \neq 0$$

The ANNNI model

$$\mathcal{H} = -J_1\sum_{i,j:nn}\sigma_i\sigma_j + J_2\sum_{i:nnn}\sigma_i\sigma_{i+2}$$

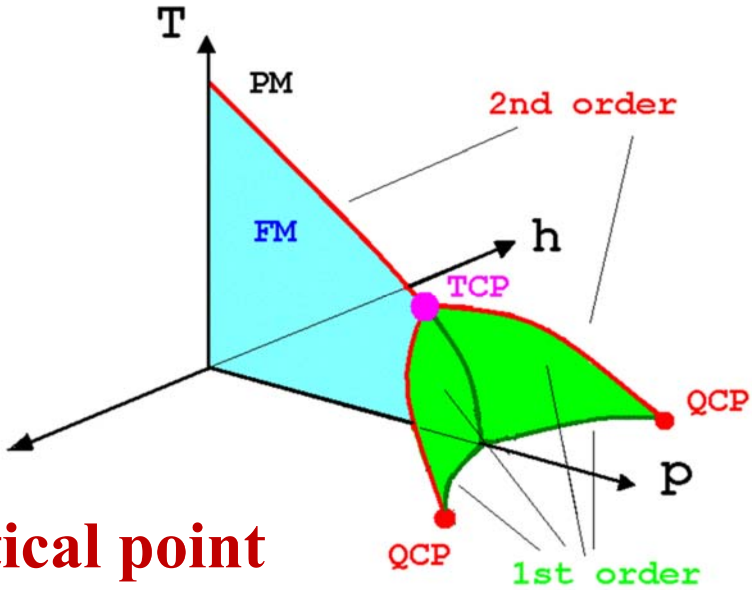




Lifshitz point

Metamagnet

$$\mathcal{H} = J_1 \sum_{i,j:nn} \sigma_i \sigma_j - J_2 \sum_{i,j:nnn} \sigma_i \sigma_j - p \sum_i \sigma_i + h \sum_i (-1)^i \sigma_i$$



Tricritical point

The O(n) model

O(n) model:

$$\mathcal{H}_{n-vector} = -J \sum_{i,j=nn} \vec{S}_i \vec{S}_j - H_1 \sum_i S_i^1 \quad \text{with} \quad \left\| \vec{S}_i \right\| = 1, \ \ \vec{S}_i = \left(S_i^1, \ldots, S_i^n \right)$$

n = 1 is the Ising model, n = 2 is the *XY*-model:

$$\mathcal{H}_{XY} = -J \sum_{i,j=nn} \vec{S}_i \vec{S}_j - H_x \sum_i S_i^x \quad \text{with} \quad \left\| \vec{S}_i \right\| = 1, \ \ \vec{S}_i = \left(S_i^x, S_i^y \right)$$

n = 3 is the Heisenberg model:

$$\mathcal{H}_{Heisenberg} = -J \sum_{i,j=nn} \vec{S}_i \vec{S}_j - H_x \sum_i S_i^x \ \ \text{with} \ \ \left\| \vec{S}_i \right\| = 1, \ \vec{S}_i = \left(S_i^x, S_i^y, S_i^z \right)$$

$n = \infty$ is the „spherical model“.

Phase transitions

Mermin-Wagner theorem (1966):

In two dimensions a system with continuous degrees of freedom and short range interactions has no phase transition which involves long range order.

Heisenberg model in three dimensions:

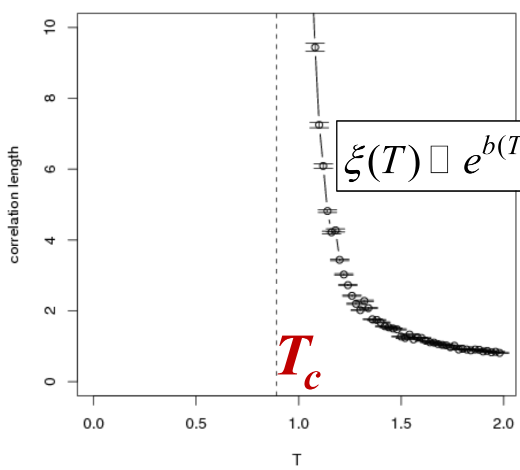
quantity	functional form	exponent	
magnetization	$m \propto (T_c - T)^{\beta}$	β	0.3639(35)
susceptibility	$\chi \propto \vert T - T_c\vert^{-\gamma}$	γ	1.3873(85)
correlation length	$\xi \propto \vert T - T_c\vert^{-\nu}$	ν	0..7048(30)
specific heat	$C(T) \propto \vert T - T_c\vert^{-\alpha}$	α	0.1144(90)
inverse critical temperature	simple cubic	$1/T_c$	0.693035(37)
	bc cubic		0.486798(12)

XY model

2 dimensions

Michael Kosterlitz

David Thouless



$$\xi(T) \sim e^{b(T_c - T)^{-\nu}}$$

below T_c :

$$\left\langle \vec{s}(\vec{x}_i)\cdot\vec{s}(\vec{x}_j)\right\rangle \sim r^{-\eta(T)} \quad , \quad r = \left|\vec{x}_i - \vec{x}_j\right|$$

KT-transition $\eta(T_c) = \dfrac{1}{4}$

XY model

No symmetry breaking, no long-range order

But still scaling behavior at T_c

correlation length:

$$\xi(T) \sim e^{b(T_c - T)^{-\nu}} \quad , \quad \nu = \frac{1}{2}$$

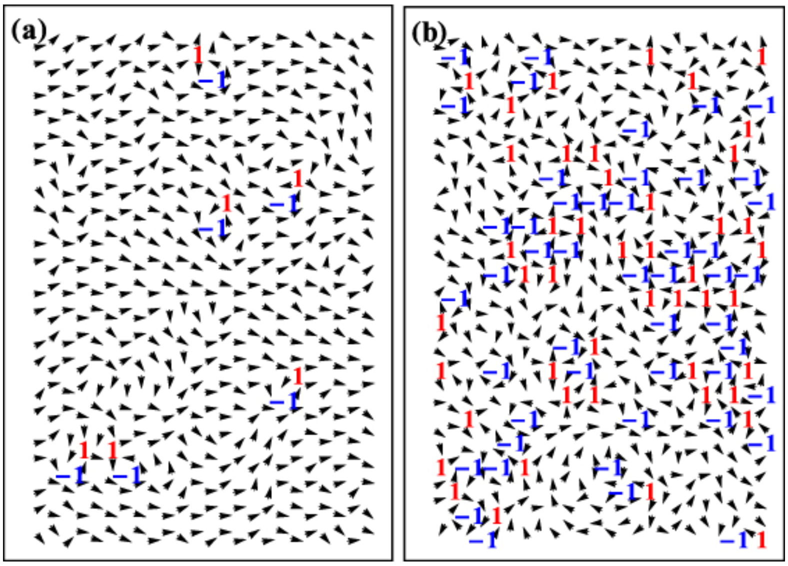
specific heat:

$$C(T) \sim \xi(T)^{-2} \left(\ln \xi(T)\right)^{-q} \quad , \quad q = 6$$

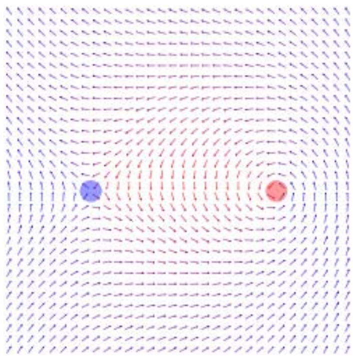
susceptibility:

$$\chi(T) \sim \xi(T)^{2-\eta_c} \left(\ln \xi(T)\right)^{-2r} \quad , \quad r \approx 0.056$$

XY model



vortex-antivortex pair



At low temperatures the vortices are bound in vortex-antivortex pairs, which dissociate at the KT transition.

Continuous degrees of freedom

Phase space is not discrete anymore.

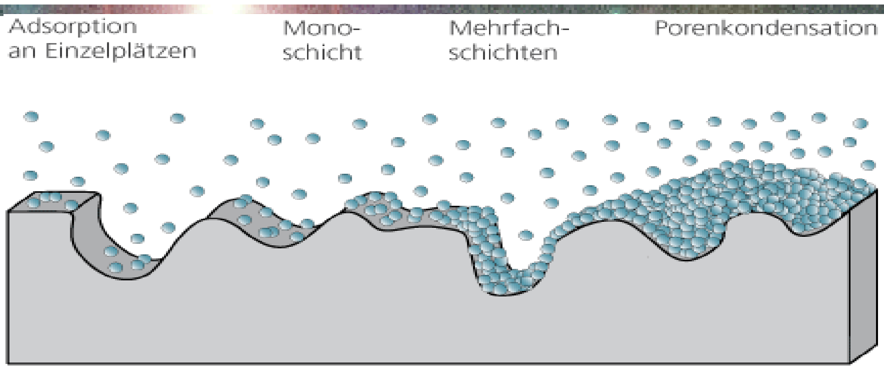
Monte Carlo move: Choose for site *i* a new spin:

$$\vec{S}_i' = \vec{S}_i + \Delta\vec{S} \quad \text{with small random } \left\|\Delta\vec{S}\right\| \;, \quad \Delta\vec{S} \perp \vec{S}_i$$

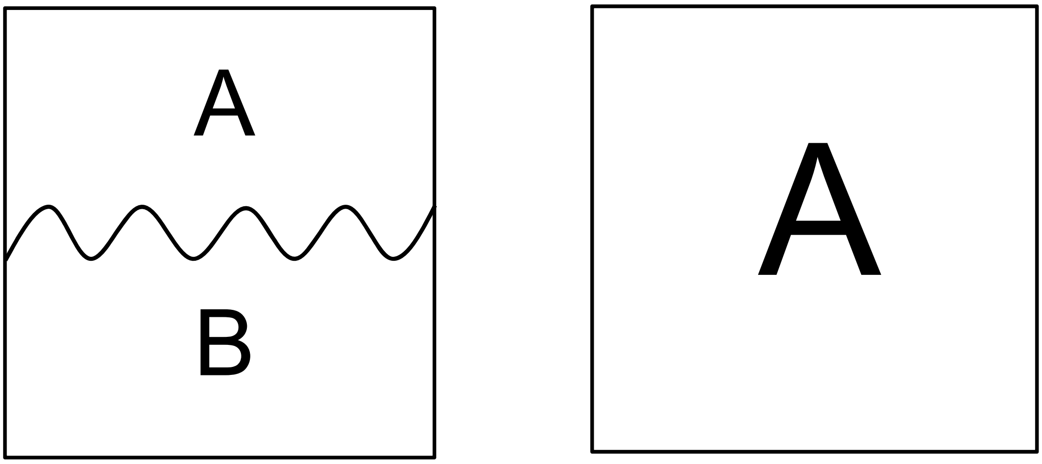
- Calculate ΔE
- Metropolis: If $\Delta E \leq 0$ flip, else flip with $p = \exp(-\beta\Delta E)$.
- Glauber: Flip with probability $p = \exp(-\beta\Delta E)/(1+\exp(-\beta\Delta E))$.

applet

Interfaces



Interfaces



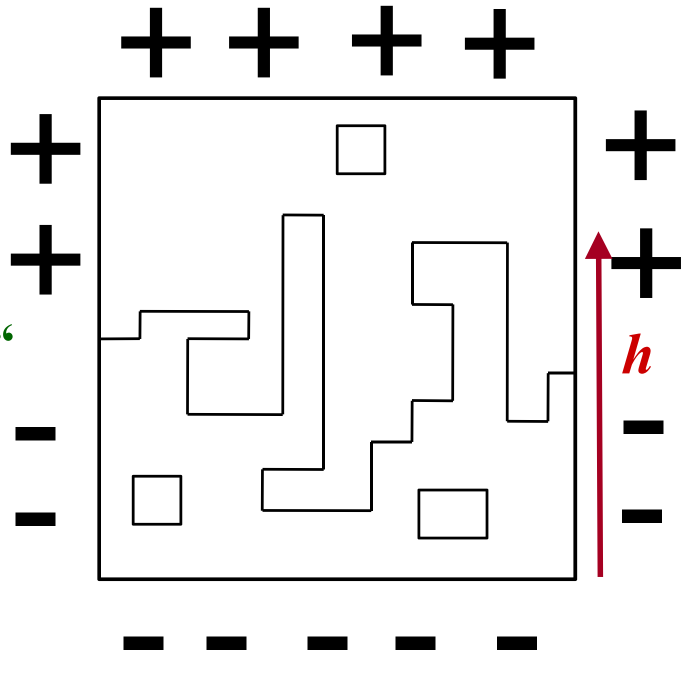
surface tension

$$\gamma = f_{\mathrm{A+B}} - f_{\mathbf{A}}$$

Ising interface

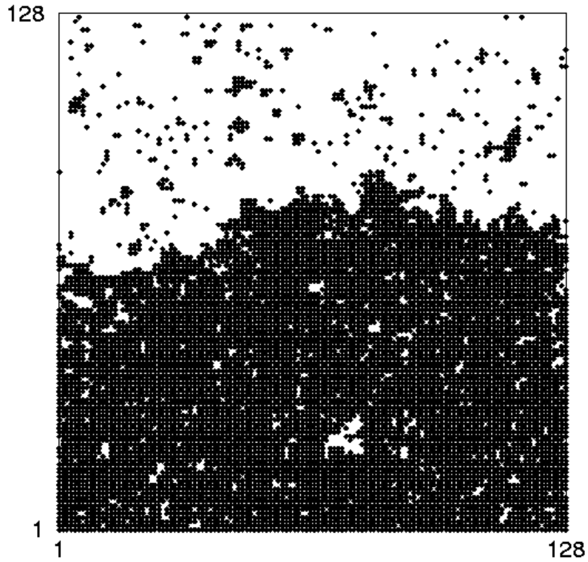
$$\mathcal{H} = \boldsymbol{E} = -\boldsymbol{J} \sum_{i,j:nn}^{N} \sigma_i \sigma_j$$

Fixed boundary conditions:
upper half „+“, lower half „–“
Simulate with Kawasaki dynamics at temperature *T*.

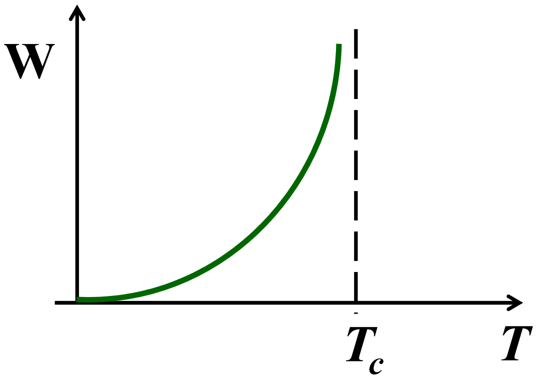


Ising interface

interface width W:



$$W = \sqrt{\frac{1}{N}\sum_i \left(h_i - \bar{h}\right)^2} \qquad \bar{h} = \frac{1}{N}\sum_i h_i$$



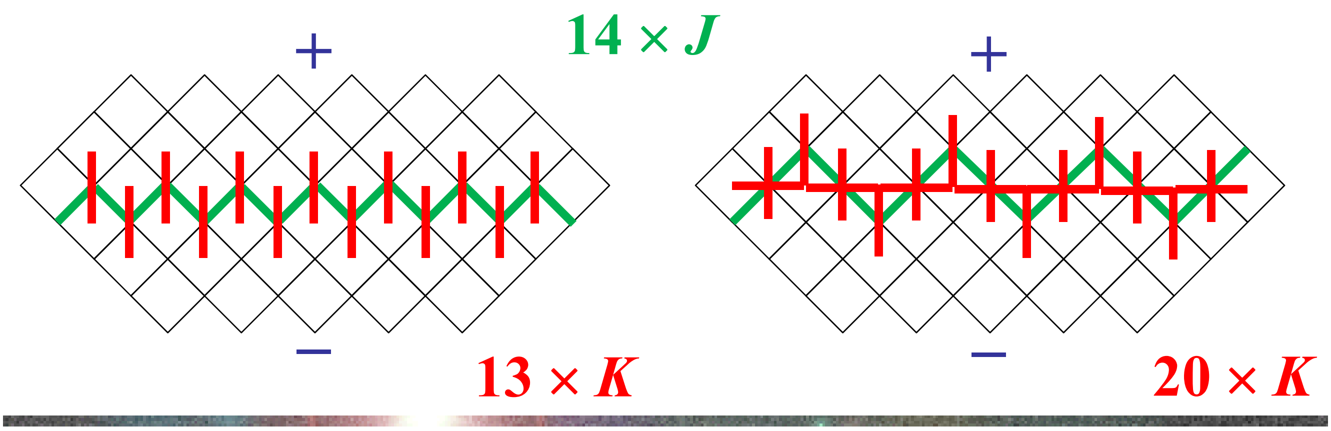
roughening transition

Ising interface

Add next-nearest neighbor interaction:

$$\mathcal{H} = \boldsymbol{E} = -\boldsymbol{J} \sum_{i,j:nn}^{N} \sigma_i \sigma_j - \boldsymbol{K} \sum_{i,j:nnn}^{N} \sigma_i \sigma_j$$

punishes curvature ↔ introduces stiffness



Shape of drop

- Start with a block of +1 sites attached to wall of an $L\times L$ system filled with -1.
- Hamiltonian including gravity g:

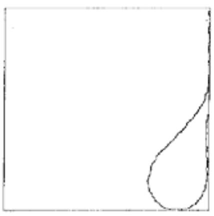
$$\mathcal{H} = E = -J\sum_{i,j:nn}^{N}\sigma_i\sigma_j - K\sum_{i,j:nnn}^{N}\sigma_i\sigma_j - \sum_j h_j \sum_{line\ j}\sigma_i$$

with $\quad h_j = h_1 + \dfrac{(j-1)(h_L - h_1)}{L-1} \quad$ and $\quad g = \dfrac{h_L - h_1}{L}$

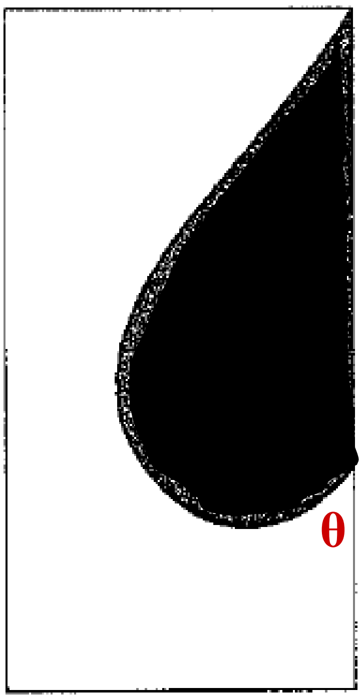
- Use Kawasaki dynamics and further do not allow for disconnected clusters of +1.

Shape of drop

$L = 257$, $V = 6613$, $g = 0.001$
after 5×10^7 MC updates
averaged over 20 samples.

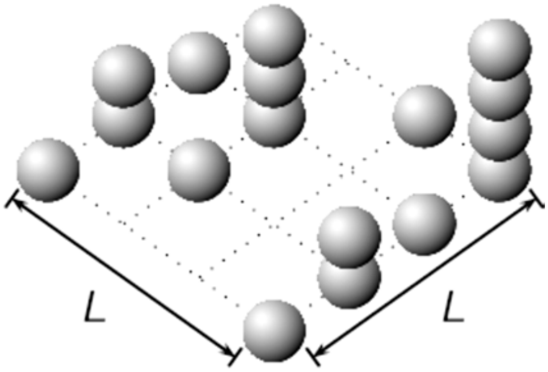


Contact angle θ is function of temperature and vanishes when approaching T_c.



Solid on solid model (SOS)

adatoms and surface growth



interface without islands and without overhangs

$$\mathcal{H} = \boldsymbol{E} = \varepsilon \sum_{i,j:nn}^{N} \left| \boldsymbol{h}_i - \boldsymbol{h}_j \right|$$

Self-affine scaling

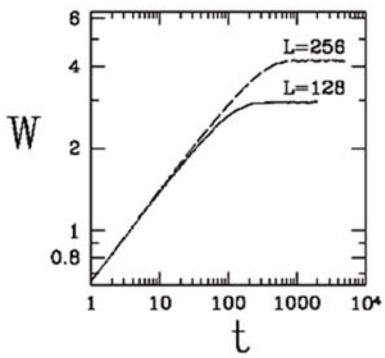


Figure 1. Interface width W versus time t for the RSOS model (Ref. [11]) in 1 + 1 dimensions, in two different lattice lengths L.

Family-Vicsek scaling (1985):

$$\mathrm{W}(L,t) = L^{\xi} f\left(t / L^{z}\right)$$

ξ is the roughening exponent, z the dynamic exponent.

Self-affine scaling

$$\boxed{W(L,t) = L^{\xi} f\left(t / L^{z}\right)}$$

$$\boxed{u = t / L^{z}}$$

$$t \to \infty : W \sim L^{\xi} \Rightarrow f(u \to \infty) = \text{const}$$

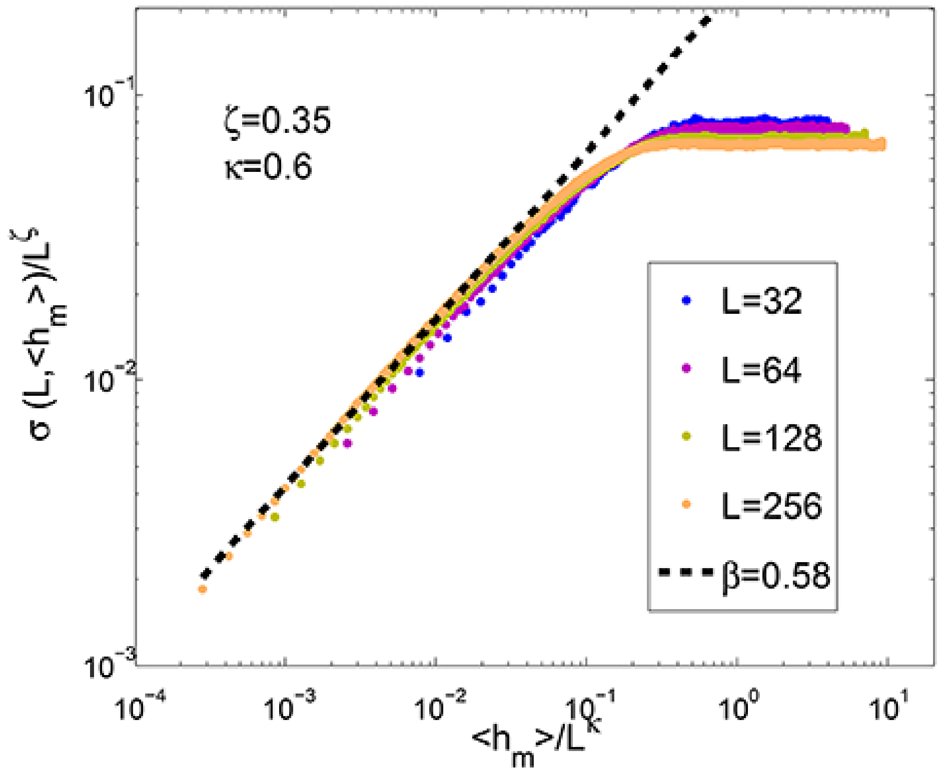
$$L \to \infty : W \sim t^{\beta} \Rightarrow f(u \to 0) \sim u^{\beta}$$

$$W \sim L^{\xi} u^{\beta} = L^{\xi}\left(t / L^{z}\right)^{\beta} = L^{\overbrace{\xi-\beta z}^{0}} t^{\beta} \Rightarrow \boxed{\beta = \frac{\xi}{z}}$$

β is the growth exponent.

Numerically these laws are verified by data collapse.

Self-affine scaling



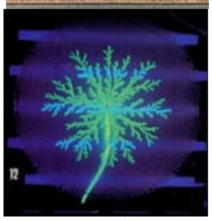
Irreversible growth

- T. Vicsek, „Fractal Growth Phenomena“ (World Scientific, Singapore, 1989
- A.-L. Barabasi and H.E. Stanley, „Fractal Concepts in Surface Growth“ (Cambridge Univ. Press, 1995)
- H.J. Herrmann, „Geometric Cluster Growth Models and Kinetic Gelation“, Phys. Rep. 136, 153 (1986)

Irreversible growth

No thermal equilibrium

- Deposition and aggregation patterns
- Fluid instabilities
- Electric breakdown
- Biological morphogenesis
- Fracture and Fragmentation


Random deposition

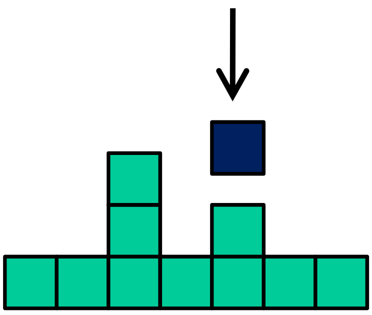
Random deposition

simplest possible growth model

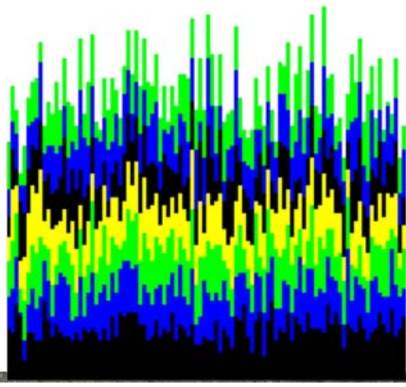
$$\langle h \rangle \sim t$$

$$W \sim t^{1/2}$$

**Pick a random column.
Add a particle on top of that column**



$$\boxed{\begin{aligned}\beta &= 1/2 \\ \xi &= 1/2\end{aligned}}$$



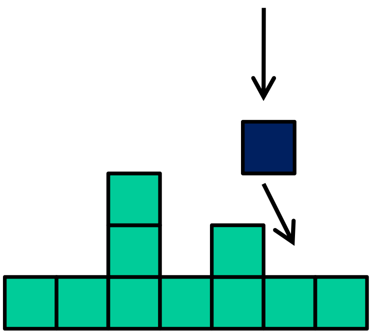
Random deposition with surface diffusion

Particle can move a short distance to find a more stable configuration.

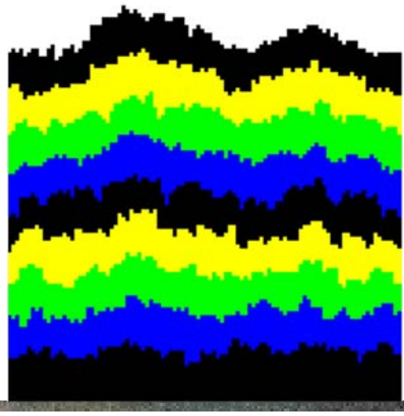
Pick a random column i.
Compare h(i) and h(i+1).
Particle is added onto whichever is lower. If they are equal, add to column i or i+1 with equal probability.

$$\langle h \rangle \sim t$$

$$W \sim t^{1/4}$$



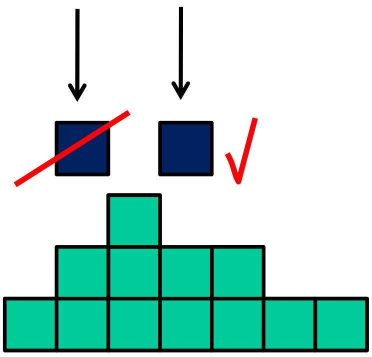
$$\boxed{\begin{array}{l}\beta = 1/4 \\ \xi = 1/2\end{array}}$$



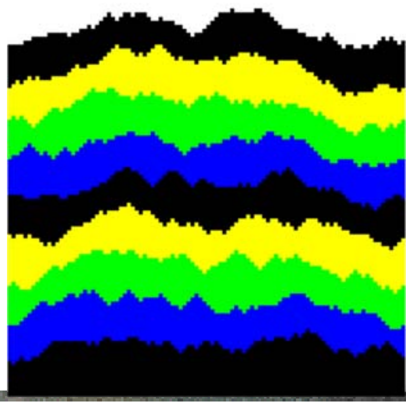
Restricted Solid On Solid Model (RSOS)

Neighbouring sites may not have a height difference greater than 1.

Pick a random column i.
Add a particle only if
h(i) ≤ h(i-1) or h(i) ≤ h(i+1).
Otherwise pick a new column.



$$\boxed{\begin{array}{l}\beta = 1/3 \\ \xi = 1/2\end{array}}$$



Growth equations

Edwards Wilkinson equation: $$\frac{\partial h(x,t)}{\partial t} = \nu \Delta h + \eta(x,t)$$

S.F. Edwards and D.R. Wilkinson (1982)

noise

$$\boxed{\beta = 1/4 \text{ and } \xi = 1/2}$$

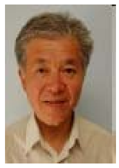
KPZ equation: $$\frac{\partial h(x,t)}{\partial t} = \nu \Delta h + \frac{\lambda}{2}(\nabla h)^2 + \eta(x,t)$$

M. Kardar, G. Parisi and Y.-C. Zhang (1986)

$$\boxed{\beta = 1/3 \text{ and } \xi = 1/2}$$


Mehran Kardar


Giorgio Parisi


Yi-Cheng Zhang

Stochastic Differential Equations


Kyoshi Itô


Ruslan L. Stratonowitsch


Martin Hairer

Itô – Stratonowitsch calculus

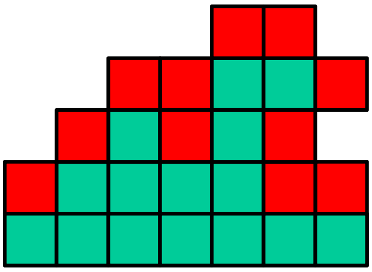
Eden model

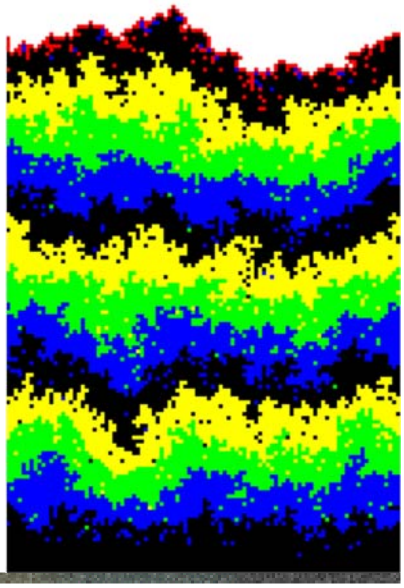
simple model for tumor growth or epidemic spread

Each site that is a neighbour of an occupied site has an equal probability of being filled.

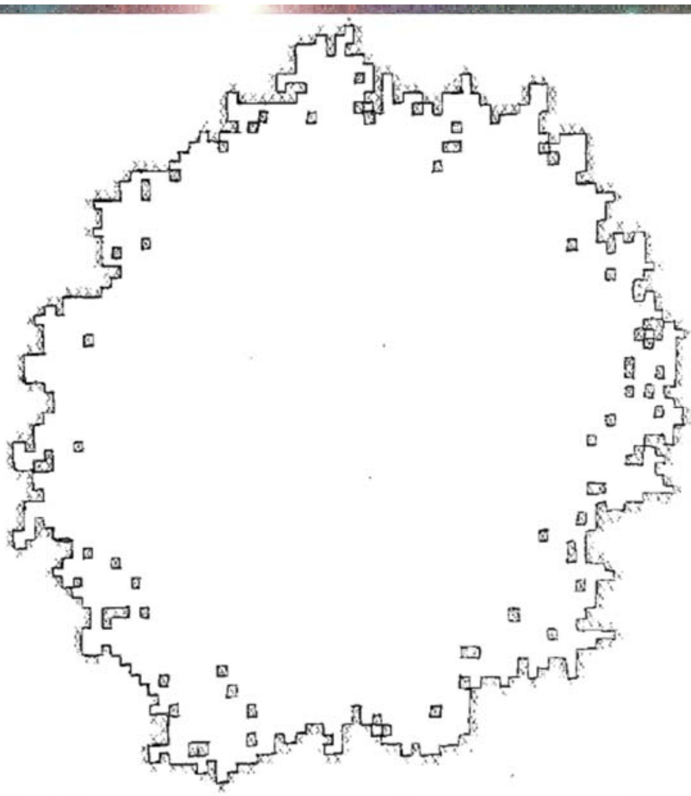
Make a list of neighbour sites (red).
Pick one at random. Add it to cluster (green).
Neighbours of this site then become red….

There can be more than one growth site in a column. Can get overhangs.





Eden cluster



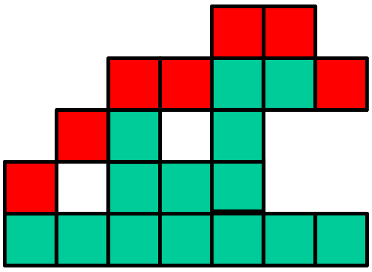
$\beta = 1/3$
$\xi = 1/2$

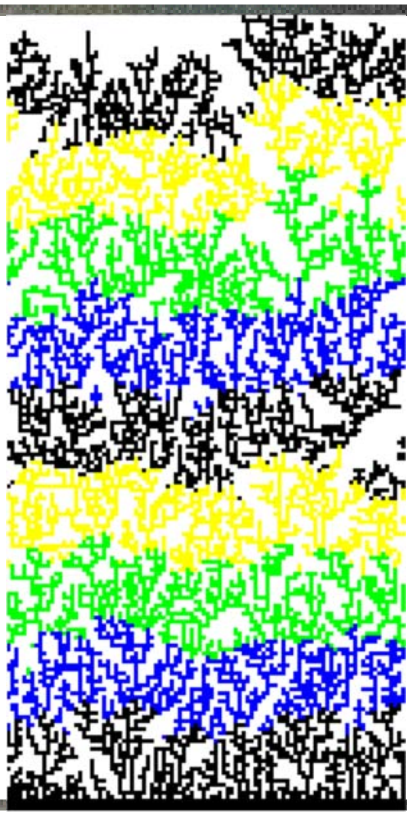
Ballistic deposition

Particles fall vertically from above and stick when they touch a particle below or a neighbour on one side.

Pick a column i. Let particle fall till it touches a neighbour. Possible growth sites are indicated in red. Only one possible site per column.

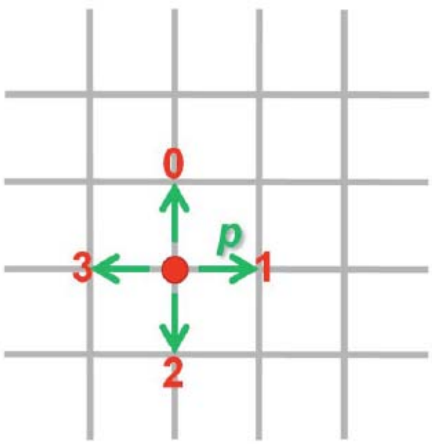
$$\beta = 1/3$$
$$\xi = 1/2$$





Random Walk

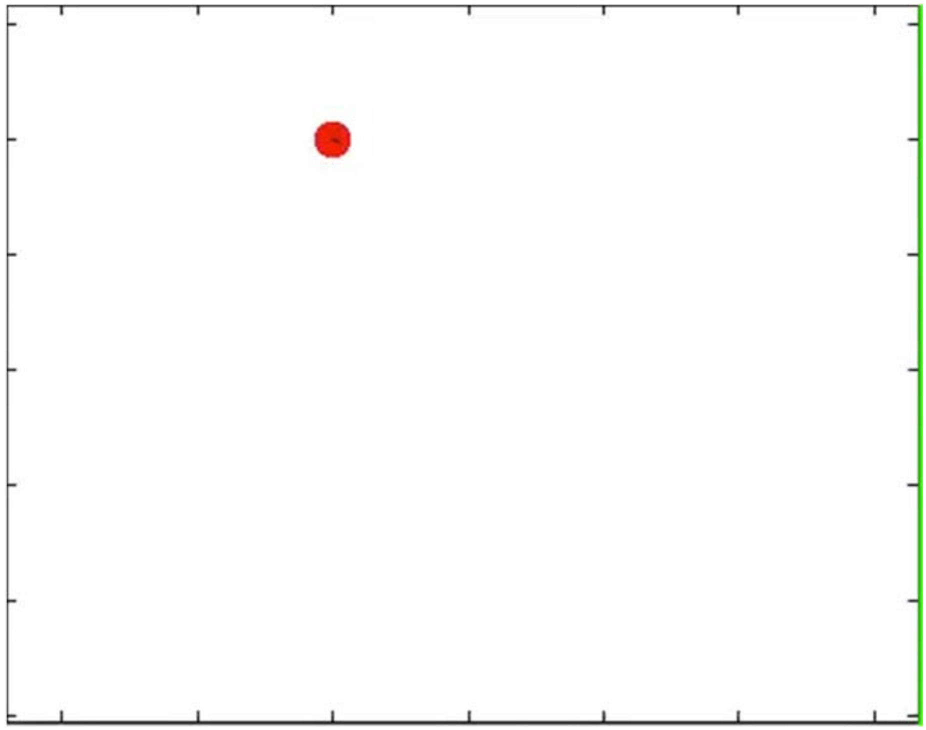
***k* = degree = number of neighbors**



$$p = \frac{1}{k}$$

Sample a random number *z* homogenously between 1 and *k* and move the walker in direction [*z*] +1, where [..] is the integer part.

Random Walk



Random Walk

The probability $p(x,t)$ to find a random walker at time t at position x is proportional to the concentration $c(x,t)$ of non-interacting random walkers (= diffusion), after ensemble averaging.

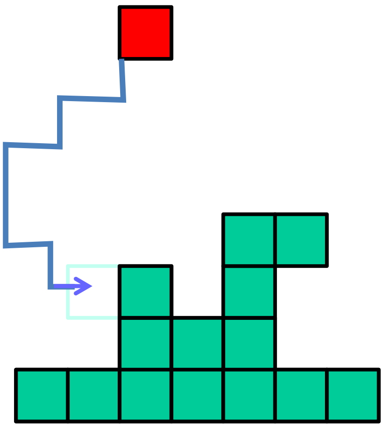
$$\boxed{\frac{\partial c(\vec{x},t)}{\partial t} = D\ \Delta c(\vec{x},t)} \qquad \boxed{\int c(\vec{x},t)dx^3 = 1}$$

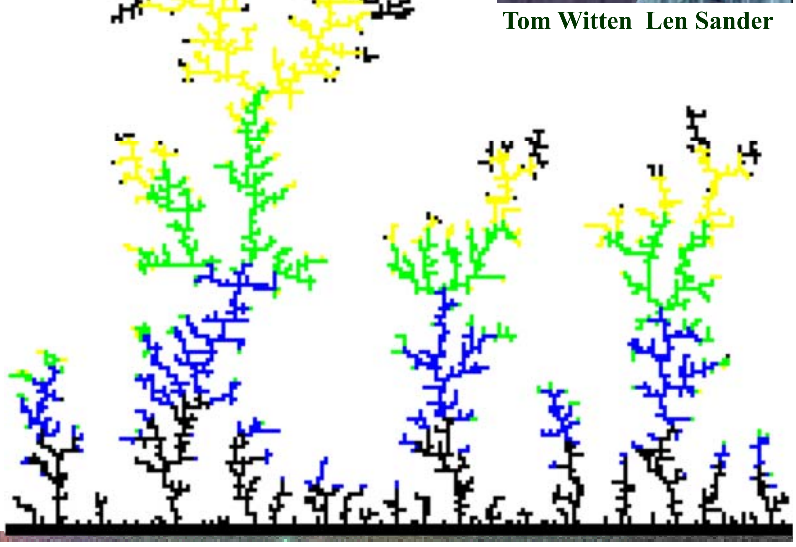
converges towards stationary solution:

$$\boxed{\Delta c(\vec{x},t) = 0}$$

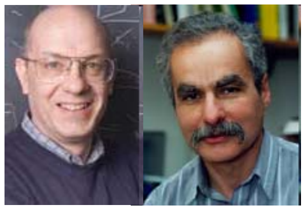
Diffusion Limited Aggregation (DLA)

A particles starts far away from surface.
It diffuses until it first touches the surface. If it moves too far away, another particle is started.



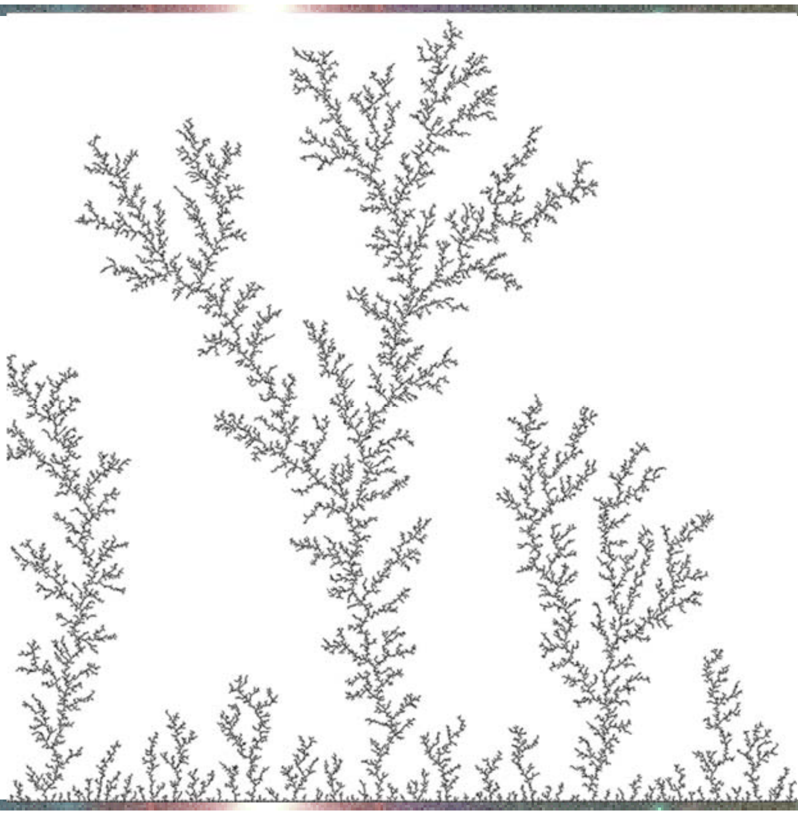


Witten and Sander, 1981



Tom Witten Len Sander

DLA clusters



fractal dimension
$d_f = 1.7$
(in 2d)

Laplacian Growth

$c_\infty = 1$

$$\Delta c(\vec{x}, t) = 0$$

growth velocity

$v_g \propto \nabla c(\vec{x}, t)$

$c_0 = 0$

$c(\vec{x}, t)$ **is the concentration of random walkers**

Laplacian Growth

$\phi_\infty = 1$

$$\Delta \phi(\vec{x}, t) = 0$$

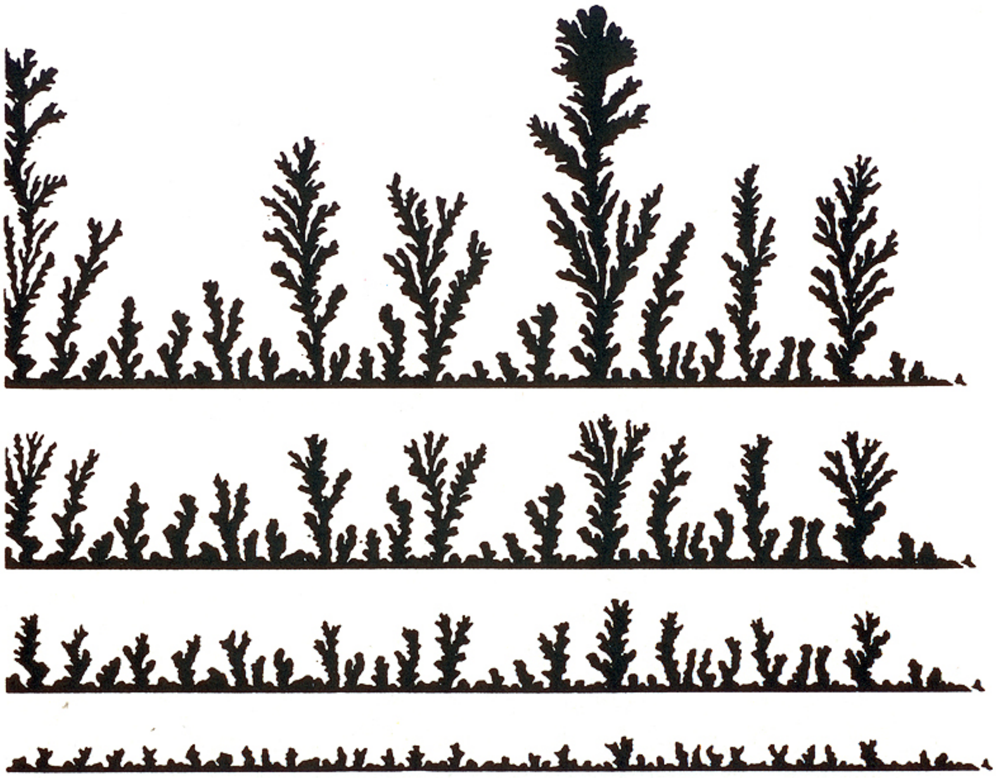
growth velocity

$v_g \propto \nabla \phi(\vec{x}, t)$

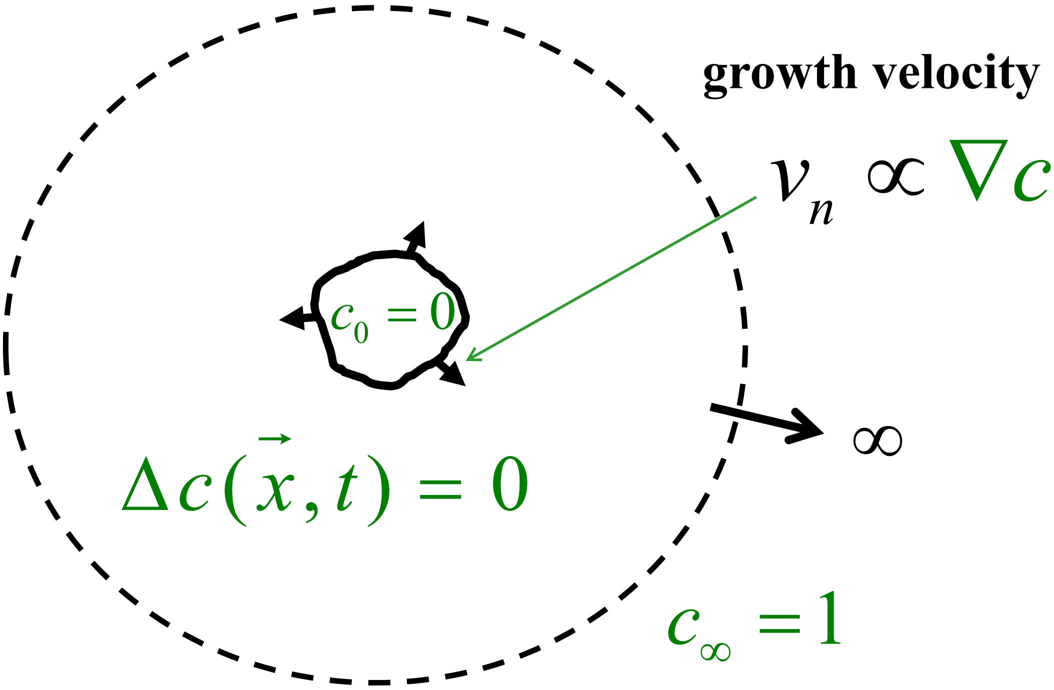
$\phi_0 = 0$

$\phi(\vec{x}, t)$ **is the electrostatic potential**

Electrodeposition

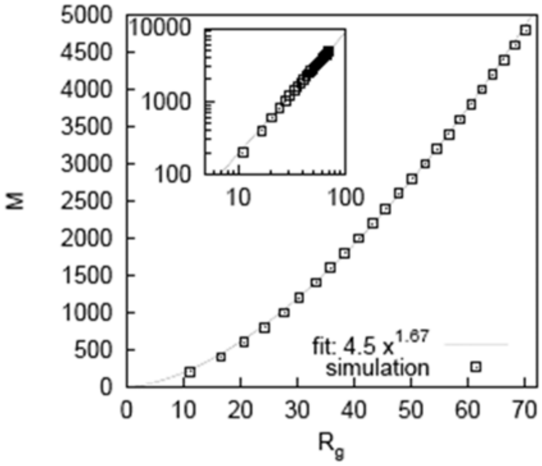


Laplacian Growth



circular geometry

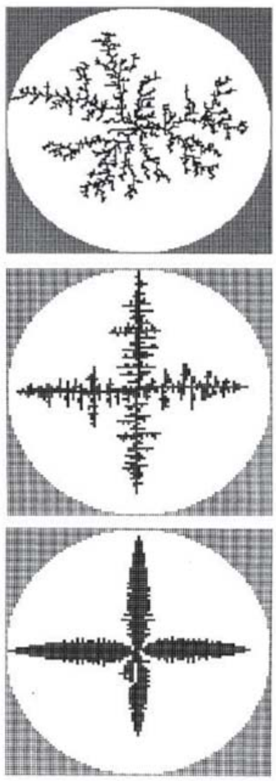
DLA clusters



anisotropy on square lattice:

Noise reduction

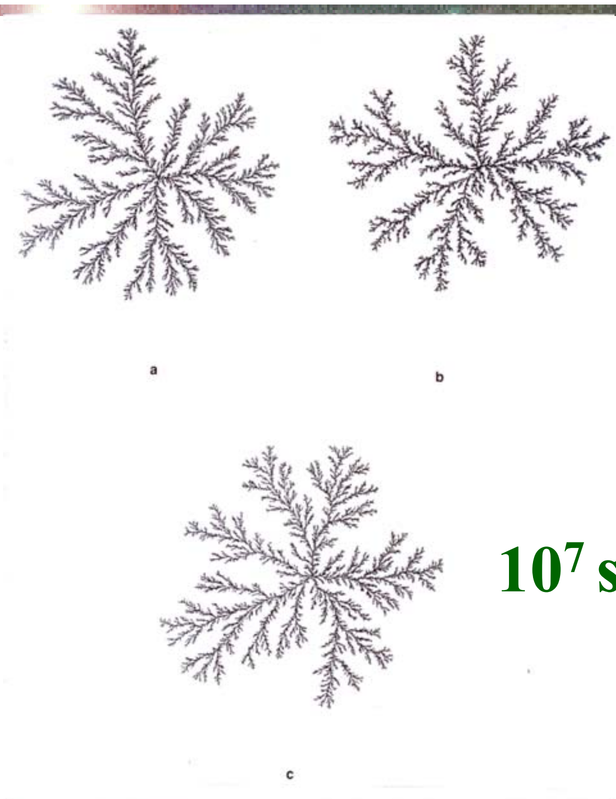
Put a counter on each site along the surface of the cluster and count how many times a random walker hits this site. only occupy the site when the number of hits reaches a certain threshold.



Self similarity

10^5 sites

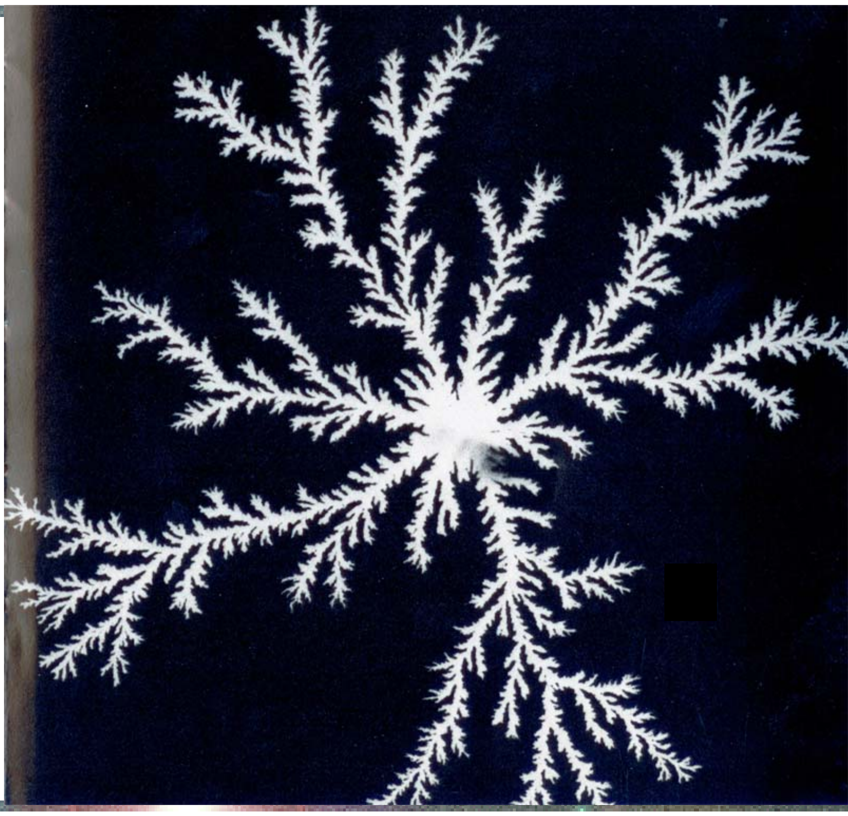
10^6 sites



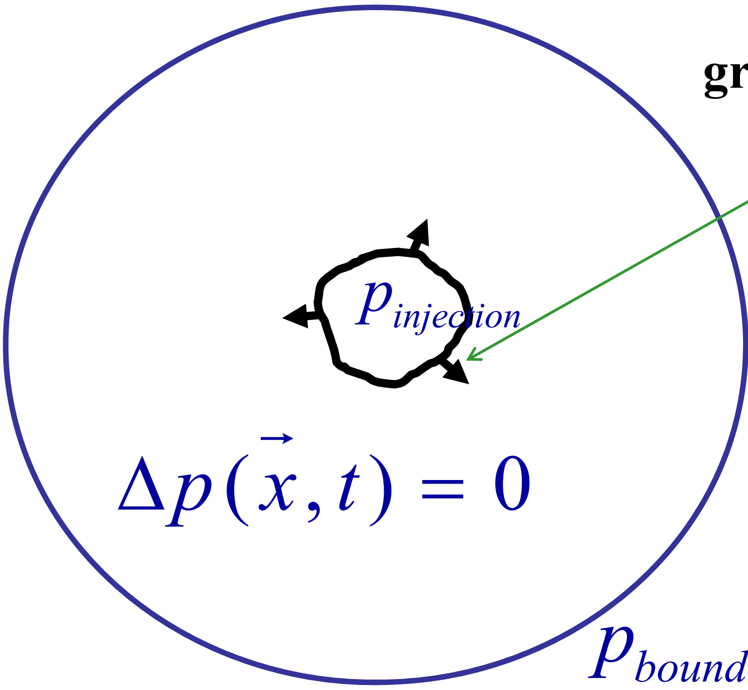
off-lattice
DLA clusters

10^7 sites

Electrodeposition



Laplacian Growth



growth velocity

$$v_n \propto \nabla p$$

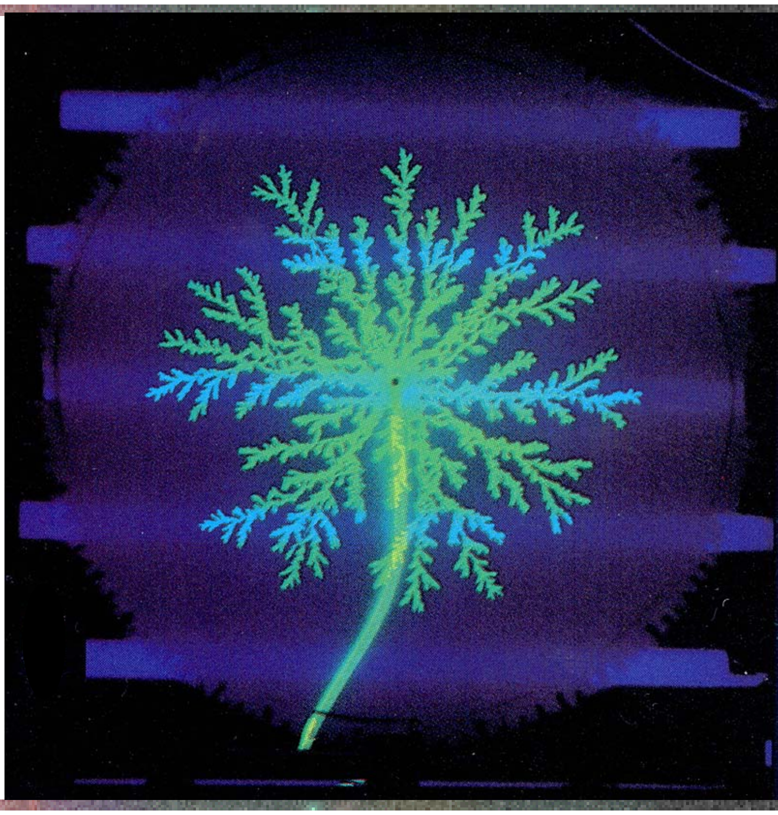
$$\Delta p(\vec{x},t) = 0$$

$$p_{boundary} < p_{injection}$$

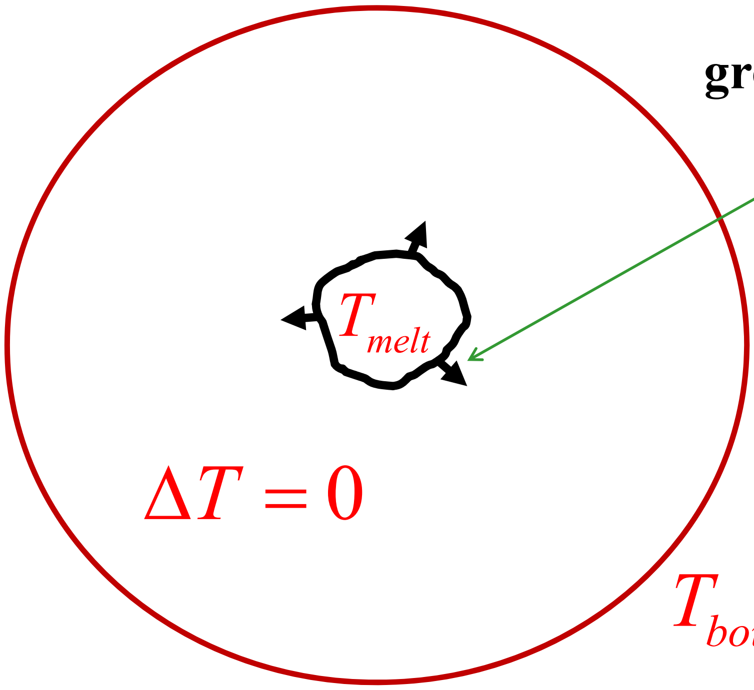
***p* (*x*,*t*) is the pressure in the Hele-Shaw cell**

Viscous Fingering

Push a less viscous fluid into a more viscous fluid inside a horizontal Hele-Shaw cell.



Laplacian Growth



growth velocity

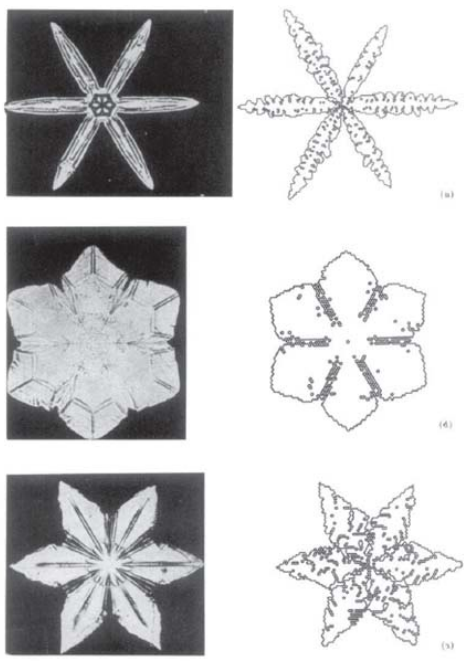
$v_n \propto \nabla T$

$T_{boundary} < T_{melt}$

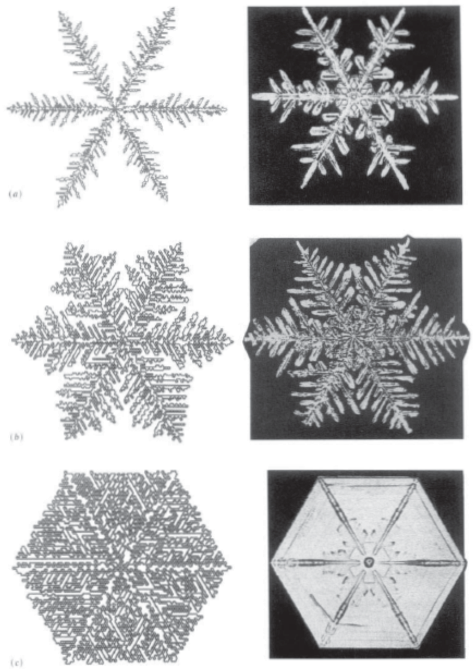
example: crystal growth inside undercooled melt

Snowflakes

real	simulation		simulation	real

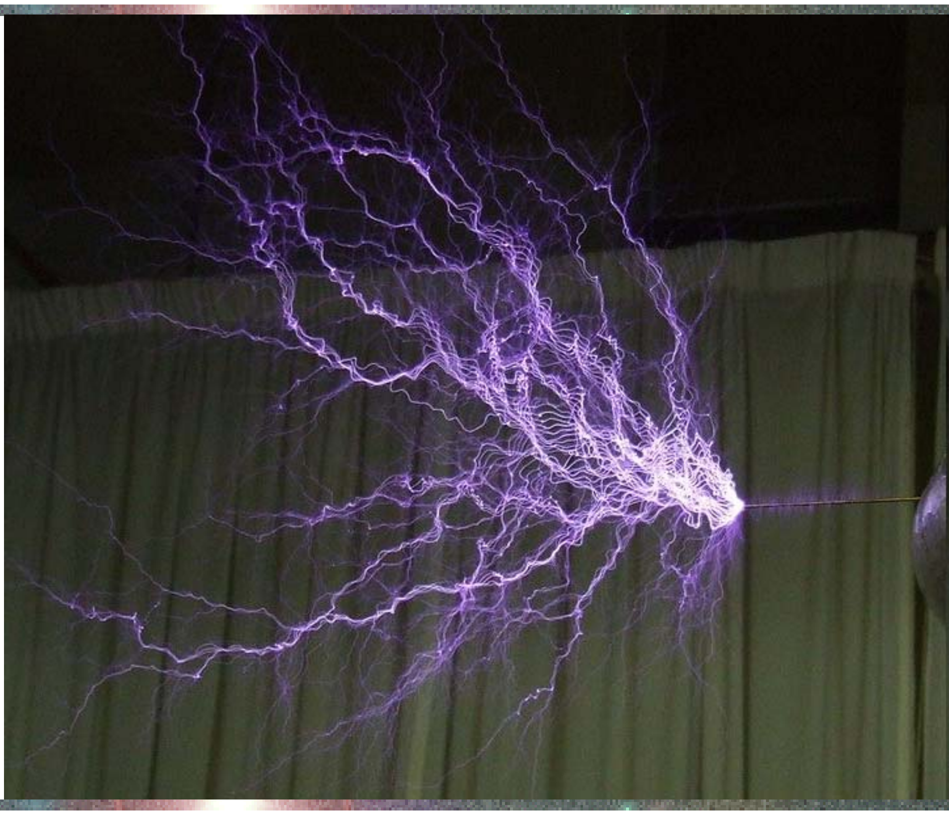


DLA with noise reduction and surface tension on the hexagonal lattice



Nittmann and Stanley, 1987

Dielectric breakdown



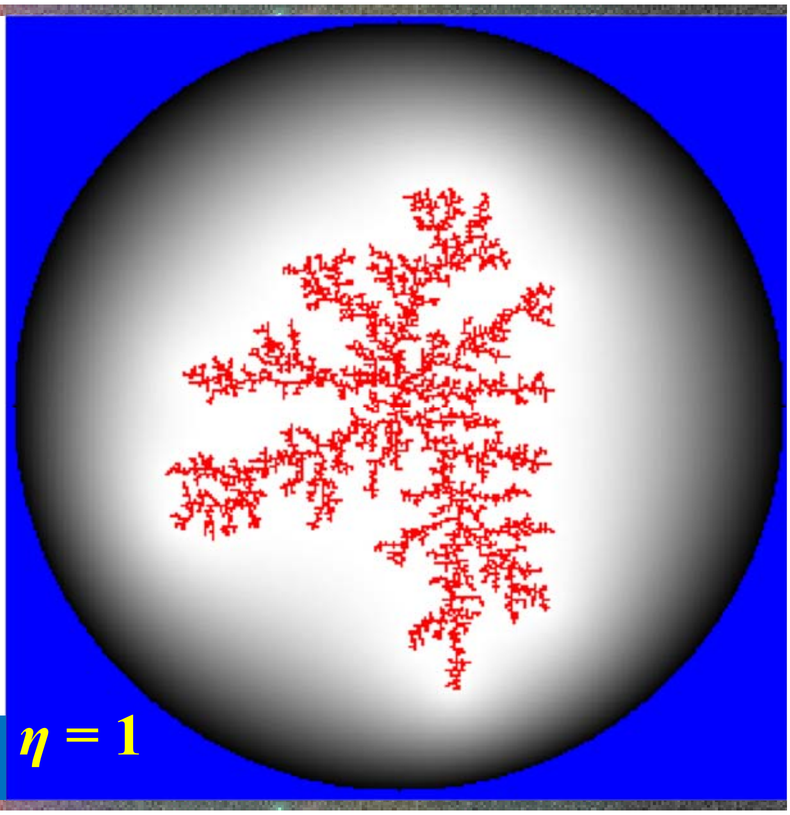
Dielectric breakdown model (DBM)

Solve Laplacian field ϕ:

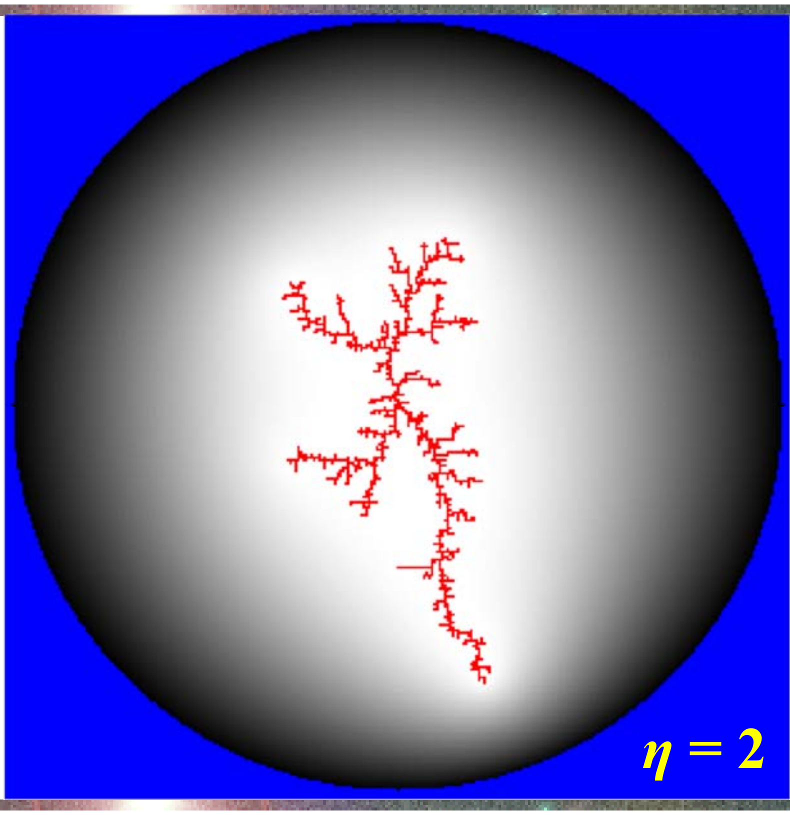
$$\boxed{\Delta\phi = 0}$$

and occupy site at boundary with probability:

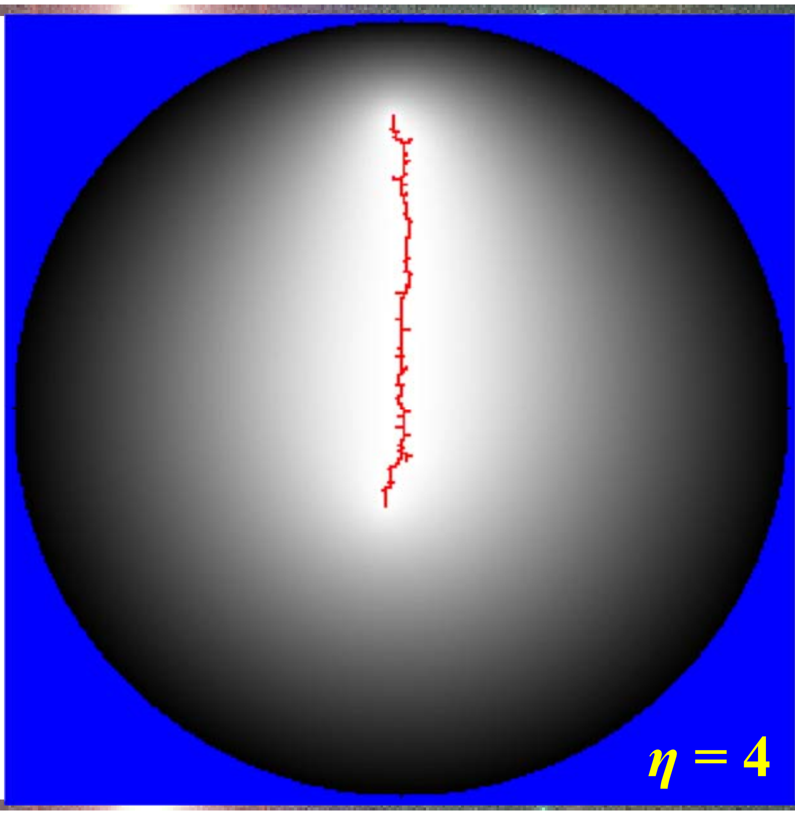
$$\boxed{p \propto (\nabla\phi)^{\eta}}$$



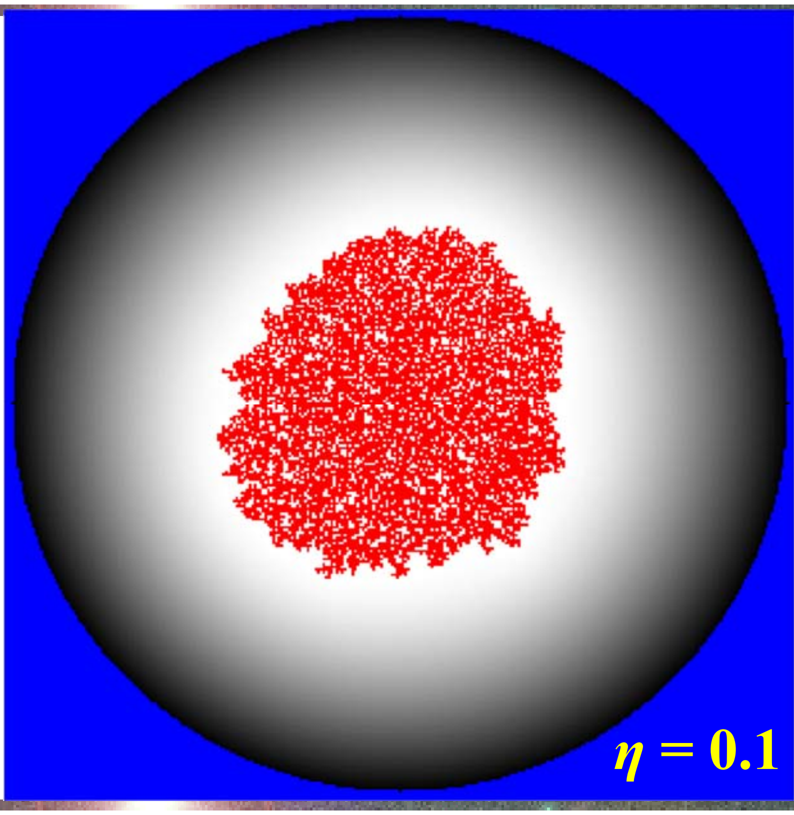
Dielectric breakdown model



Dielectric breakdown model

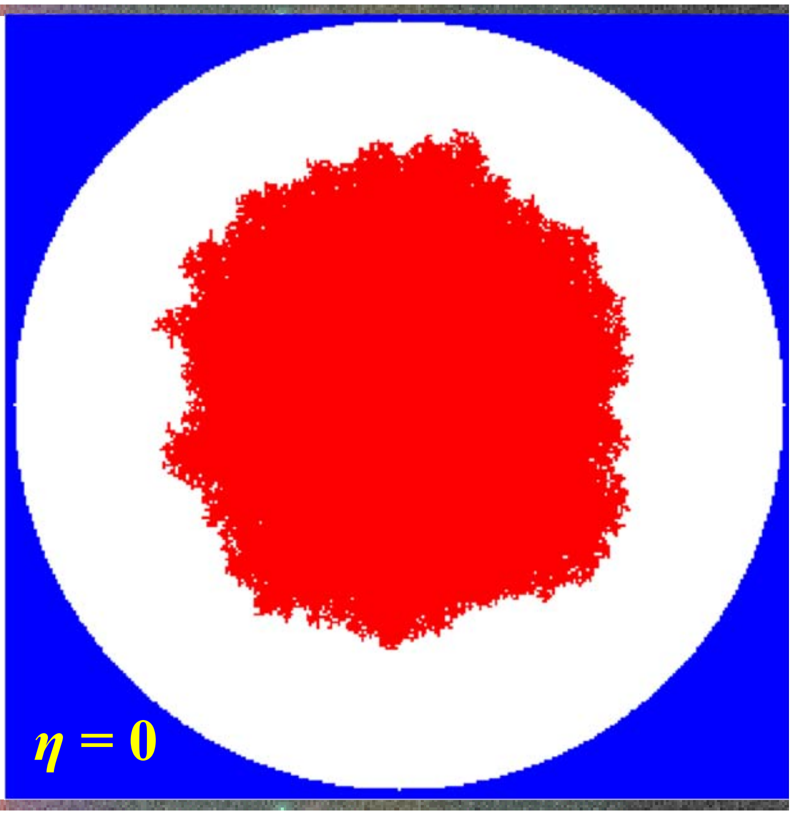


Dielectric breakdown model

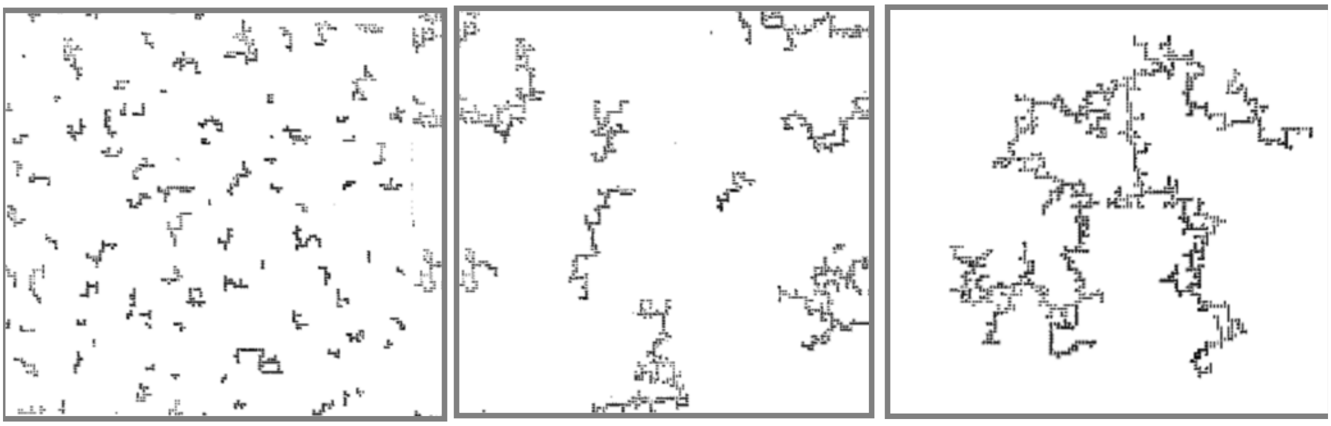


Dielectric breakdown model

same as Eden model



Clustering of clusters

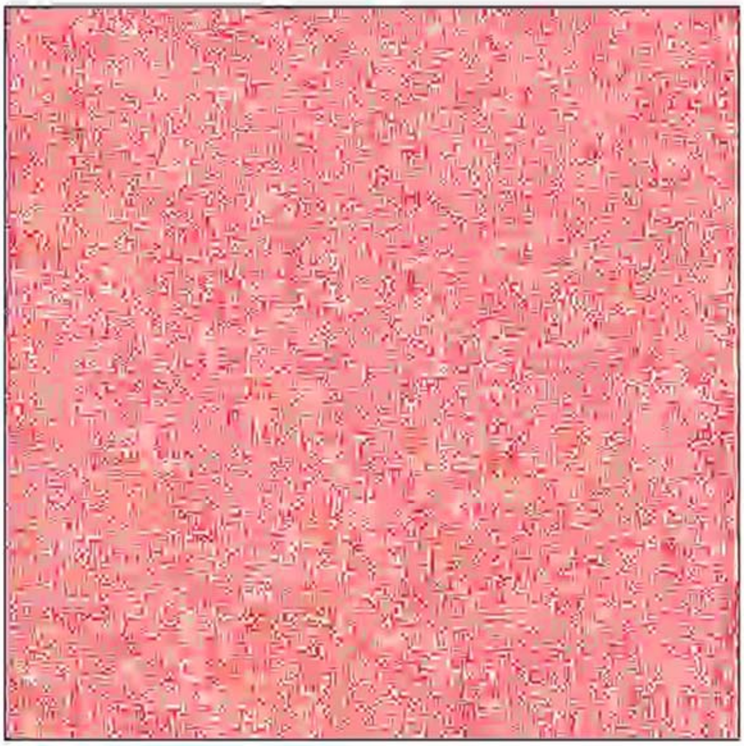


Fractal dimension is $d_f \approx 1.42$ in 2d, $d_f \approx 1.7$ in 3d.

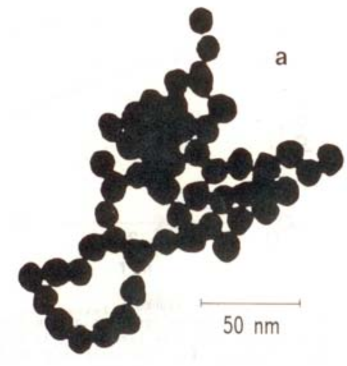
dynamical scaling: $\boxed{n_s = s^{-2} f\left(s / t^{z}\right)}$

with dynamical exponent z .

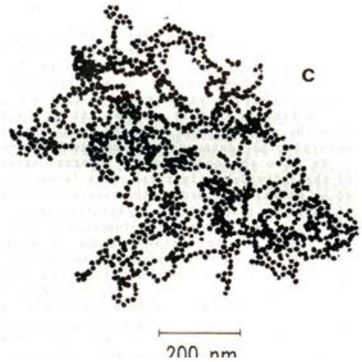
Clustering of clusters

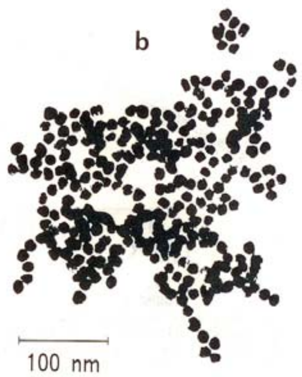


Gold colloids

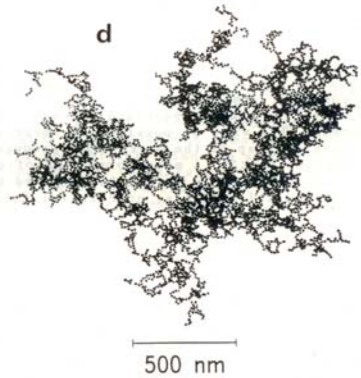


$d_f = 1.70$

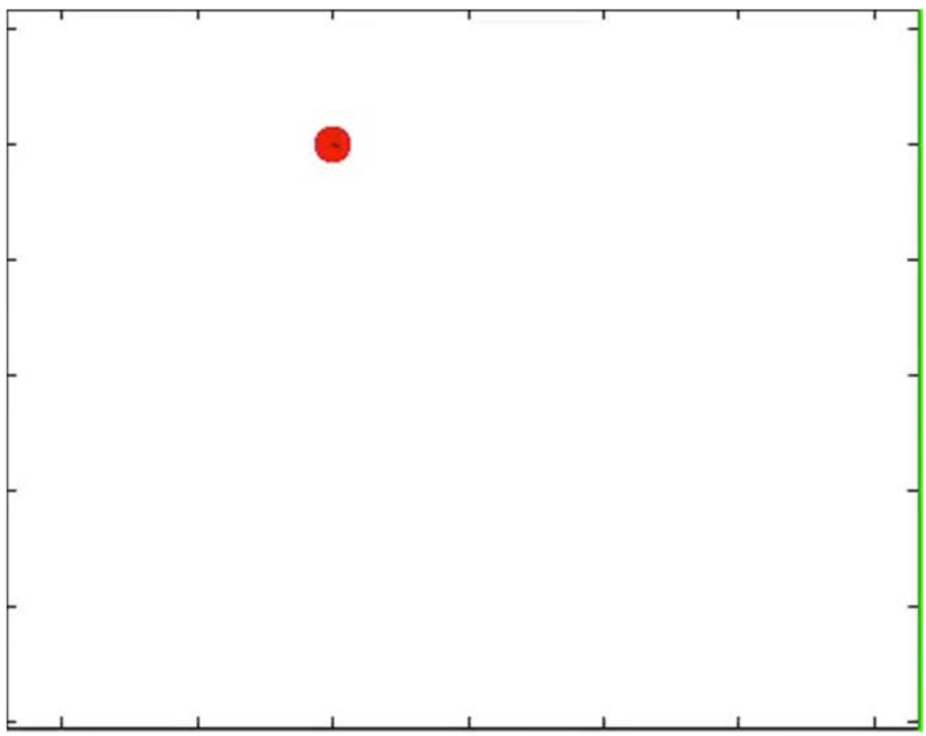




David Weitz, 1984



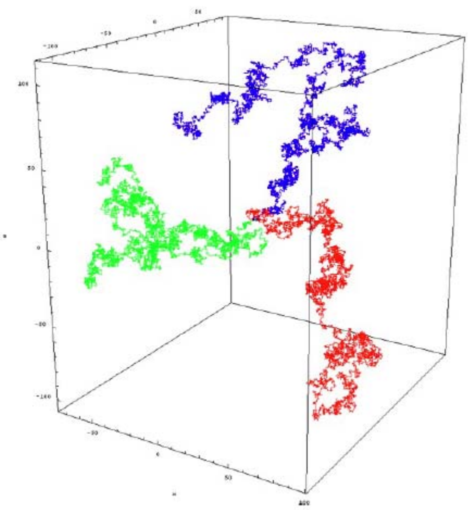
Random Walk



Application of Random Walk

- Brownian motion
- Diffusion – heat transport - pollutants
- Foraging – search algorithms
- Mathematics (SLE)
- Finance of gambling
- Polymer at theta point
- ...

Random Walk



$$X_t = X_0 + \sum_{j=1}^{t} Z_j$$

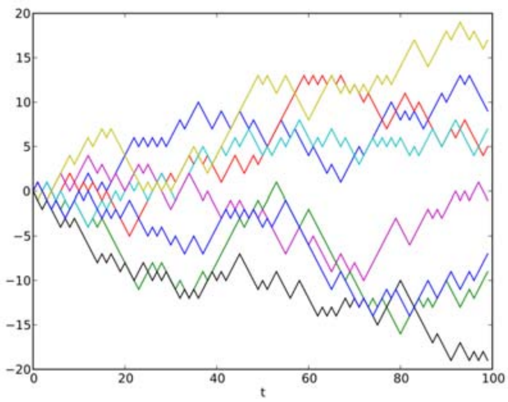
$$\left\langle x^2(t) \right\rangle = 2Dt$$

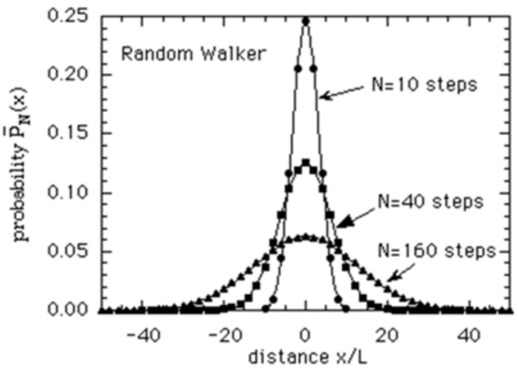
$$P(x,0) = \delta(x)$$

$$P(x,t) = \frac{N}{\sqrt{4\pi Dt}} e^{-\frac{x^2}{4Dt}}$$

central limit theorem

Random Walk

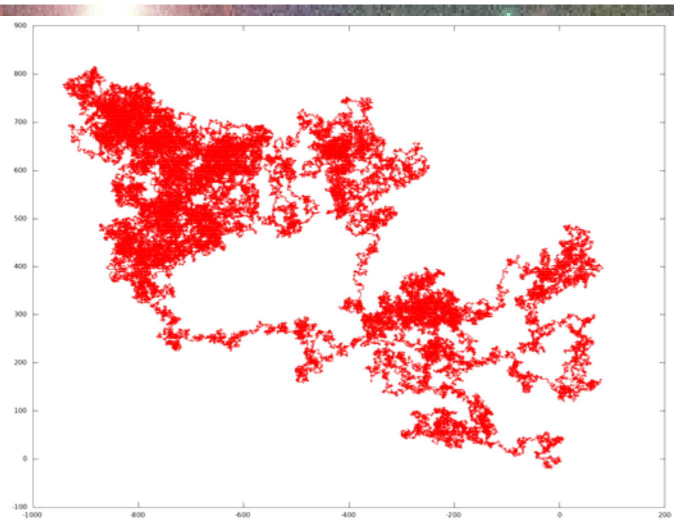




diffusion: $$\boxed{\frac{\partial c(\vec{x},t)}{\partial t} = D\ \Delta c(\vec{x},t)}$$

$$\boxed{\left\langle \vec{x}^{\,2}(t) \right\rangle = \int \vec{x}^{\,2} c(\vec{x},t) dx^3 = 2Dt}$$

Random Walk



$$\boxed{length^2 = \left\langle x^2(t) \right\rangle = 2Dt \propto mass}$$

fractal object with $d_f = 2$ in all dimensions ≥ 2

Random Walk

d-dimensions random walk

Number of visited sites (N_{cov})

$d = 1 \longrightarrow \boxed{N_{cov} \sim \sqrt{t}}$ returns with p=1

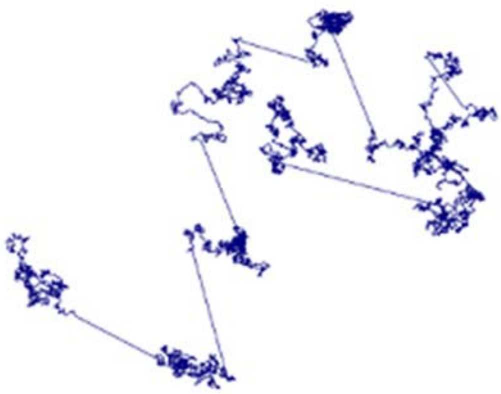
$d = 2 \longrightarrow \boxed{N_{cov} \sim t/\log(t)}$ returns with p=1

$d > 2 \longrightarrow \boxed{N_{cov} \sim t}$ may never return (w/ p>64%)

Variants of Random Walks

anomalous diffusion: $$\boxed{\left\langle x^2(t) \right\rangle = 2Dt^{\nu}}$$

Levy flights



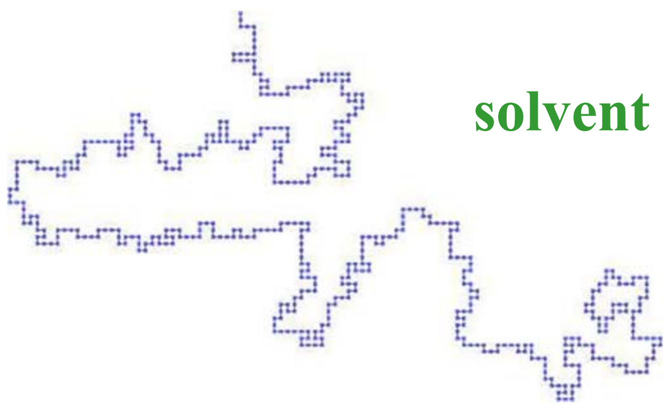
Polymers

- M.Doi, «Introduction to Polymer Physics», Clarendon Press, Oxford, 1995
- P.G. De Gennes, «Scaling Concepts in Polymer Physics», Cornell Univ. Press, 1979
- P.D. Gujrati and A.I. Leonov, «Modelling and Simulations in Polymers», Wiley, 2010
- M.Kröger, «Introduction to Computational Physics», site of IfB, ETH Zürich

Self-avoiding walk (SAW)

dilute polymer chains in good solvent

excluded volume effect



solvent

Paul Flory

N is chain length = number of monomers = degree of polymerization

Self-avoiding walk

All configurations of same chain length *N* have the same statistical weight.

number of SAW of length *N*: $\Omega_N \sim \mu^N N^\theta$

generating function:
(grand canonical partition function)

$$Z(x) = \sum_N \Omega_N x^N = \sum_N (\mu x)^N N^\theta$$

fugacity

average chain length

$$\langle N \rangle = \left.\frac{\partial \ln Z}{\partial x}\right|_{x=1} = \frac{\sum_N N\Omega_N}{\sum_N \Omega_N} = \begin{cases} \text{finite for } x < x_c \\ \text{critical at } x_c \\ \text{infinite for } x_c < x \end{cases}$$

critical fugacity

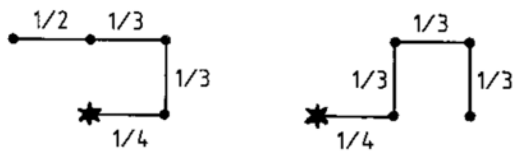
$$x_c = \frac{1}{\mu}$$

$$Z(x) = |x - x_c|^{-1-\theta}$$

Self-avoiding walk

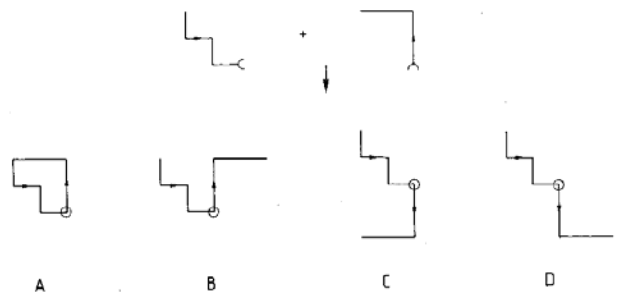
How to sample correctly self-avoiding walks?

Kinetic Growth Walk (KGW): grow a path starting from one site moving randomly to one of the empty neighbors



Dimerization:

(Alexandrowicz, 1969)



Self-avoiding walk

ETH

reptation algorithm

T. Wall and F. Mandel (1975)

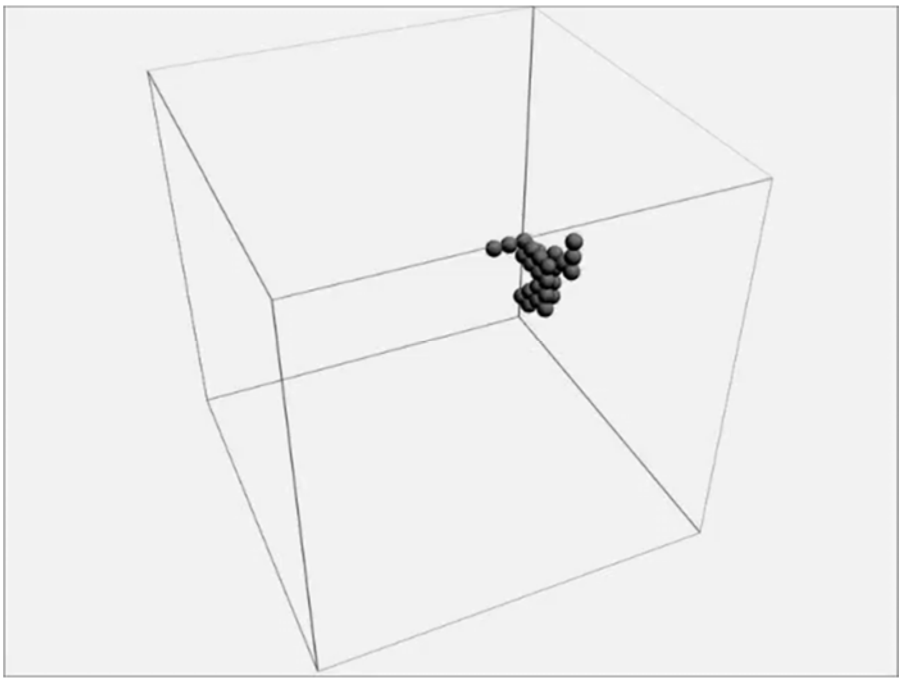
- Start with any SAW of length N
- Put the last monomer of one end in a random direction at the other end.
- If there is no overlap retain this configuration, otherwise reject the move.
- Choose randomly one end and repeat.

Simulate fixed sizes.

Self-avoiding walk

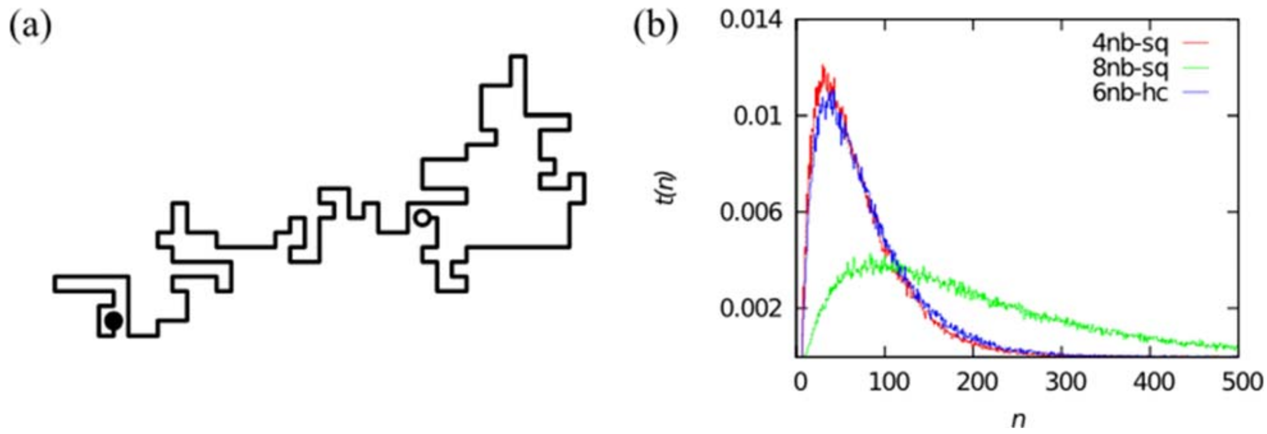
ETH

reptation algorithm



Self-avoiding walk

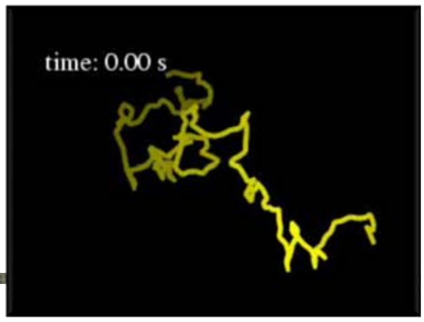
trapped configurations



Self-avoiding walk

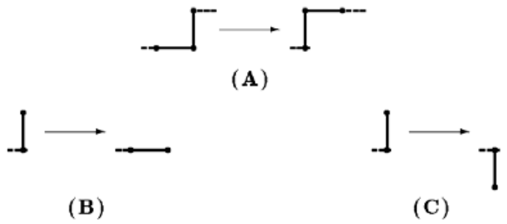
kink-jump algorithm

- **Start with any SAW of length *N***
- **Select one monomer randomly and move it to a possible (i.e. without disrupting the chain) random position.**
- **If this position is not occupied accept this move, otherwise reject.**
- **Repeat many times.**

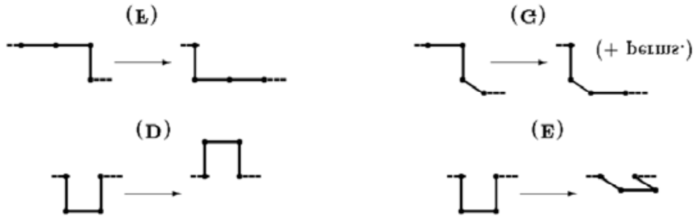


Self-avoiding walk

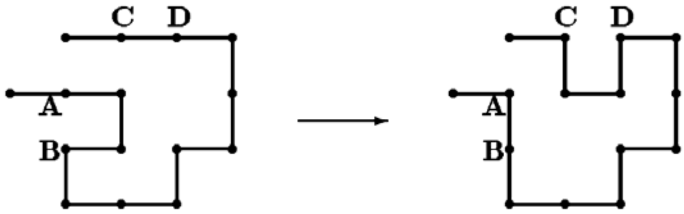
local moves involving only one monomer:



local moves involving two monomers:



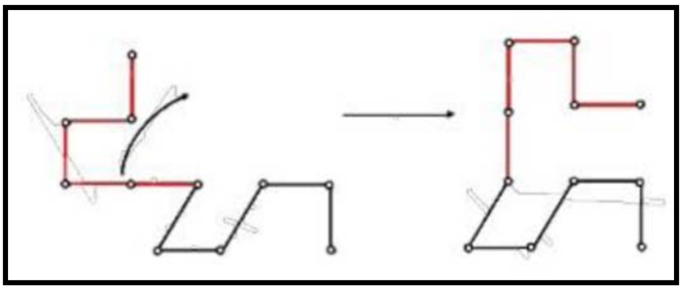
non-local move:



Self-avoiding walk

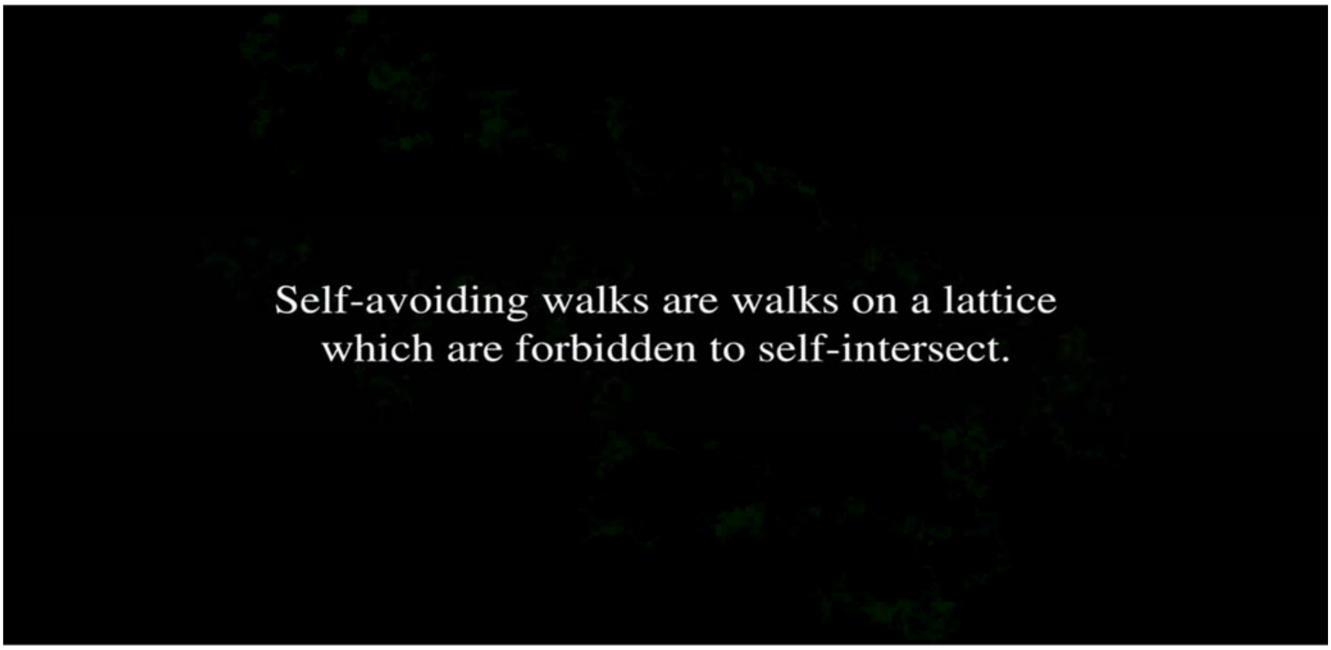
pivot algorithm N. Madras and A.D. Sokal (1988)

- Start with any SAW of length *N*.
- Select one monomer randomly as pivot.
- Perform one one branch of this pivot a transformation symmetry.
- If this produces no overlap accept this move, otherwise reject.
- Repeat many times.



Self-avoiding walk

$N = 10^8$ with pivot algorithm



Ensemble method

Take self-avoiding walk of N monomers.

Define „radius of gyration“ R_g:

$$\boxed{R_g = \frac{1}{N(N-1)}\sqrt{\sum_{i\neq j}(\vec{r}_i - \vec{r}_j)^2}}$$

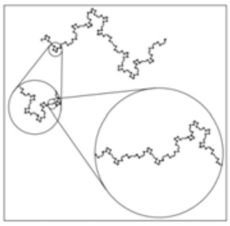
$$\boxed{N \propto R_g^{\,d_f}}$$

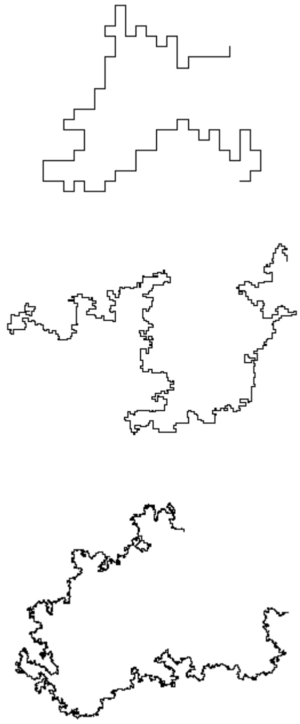
Self-avoiding walk

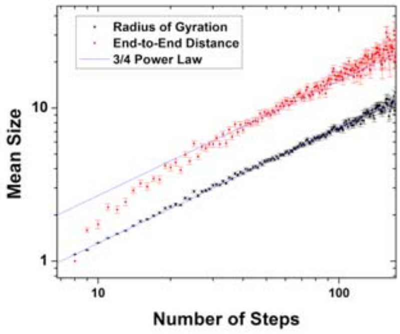
fractal dimension d_f = 4/3 in 2d

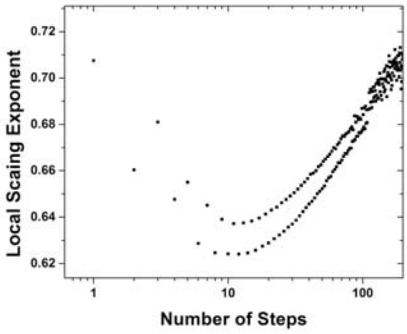
3d: $d_f \approx$ 1.701..

and d_f = 2 for d > 4.

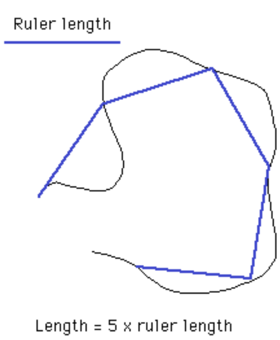


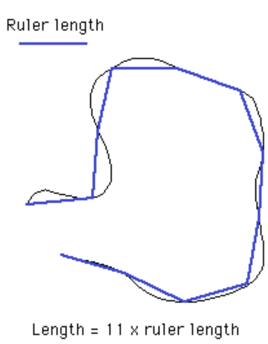


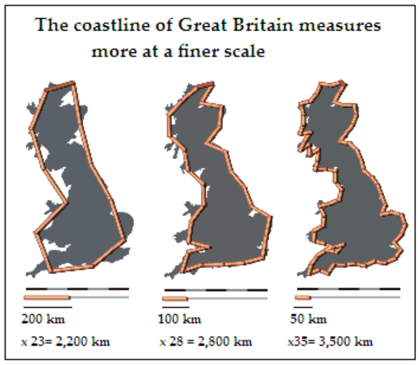


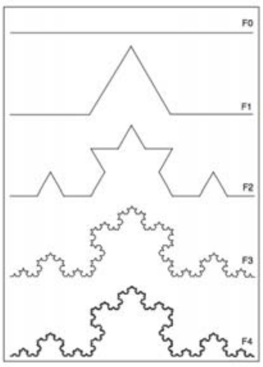


Yardstick method

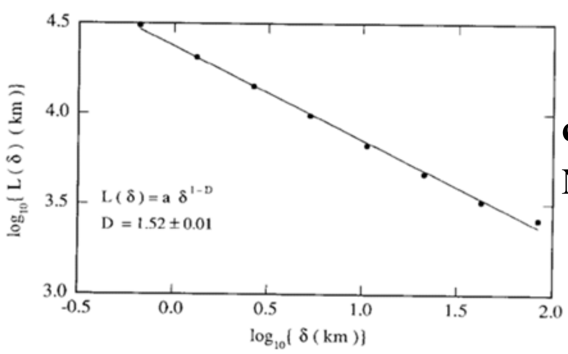






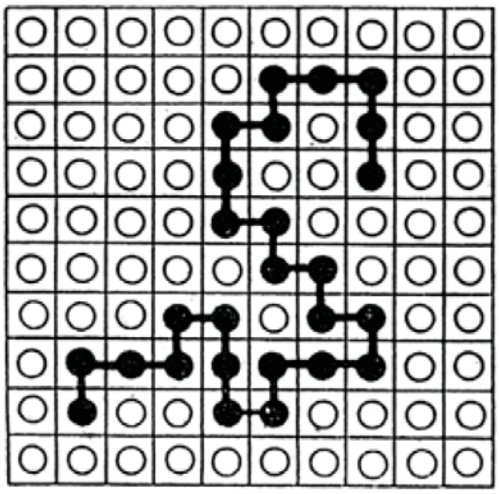


Koch curve



coast of Norway

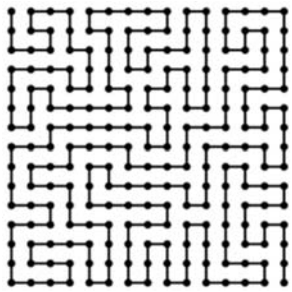
SAW with attractive interaction



$$E = -\sum_{i=1}^{N-1}\sum_{j=i+1}^{N} c_{ij} \quad , \quad c_{ij} = \begin{cases} \varepsilon & \text{if } \left|\vec{r}_i - \vec{r}_j\right| = 1 \\ 0 & \text{otherwise} \end{cases}$$

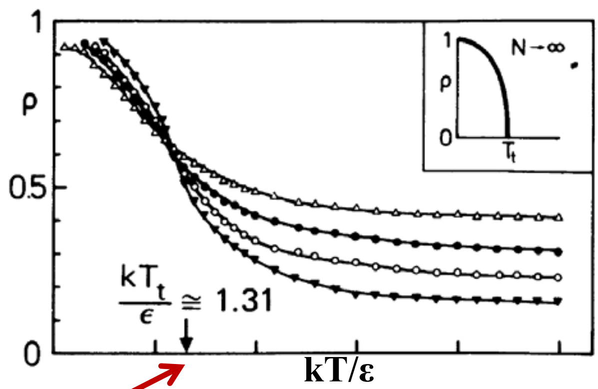
$$p(walk) = \frac{1}{Z_N} e^{-\frac{E}{kT}} \quad , \quad Z_N = \sum_{\{walks\}} e^{-\frac{E}{kT}}$$

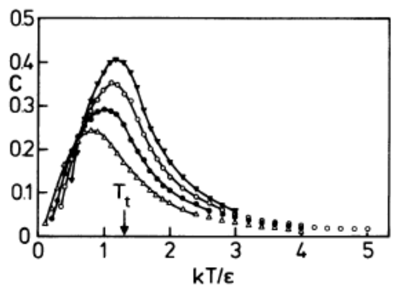
many ground states



SAW with attractive interaction

collapse of the polymer below temperature T_t





θ – point

At temperature T_t, i.e. at the θ – point, the polymer behaves like a random walk: $N \sim (R_g)^2$

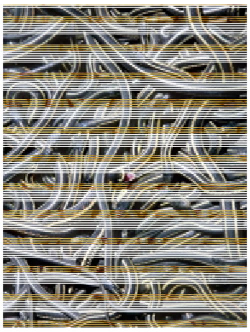
SAW with persistence

semi-flexible polymer

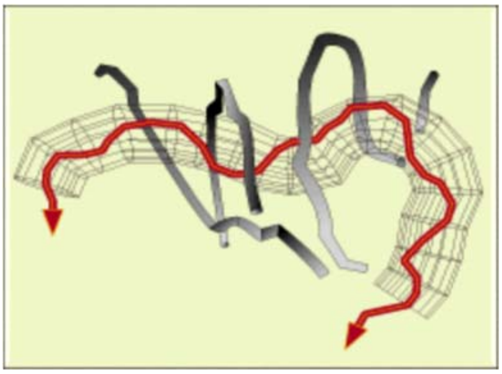
Correlation between direction of first step and nth step decays exponentially with n and the characteristic length is called «persistence length».

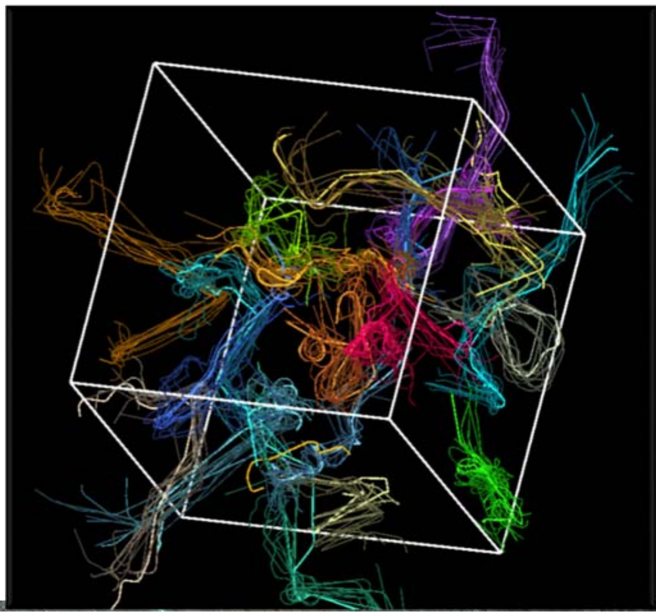
By giving more weight to straight sections than to curved ones, one can introduce an effective stiffness.

Polymer melts



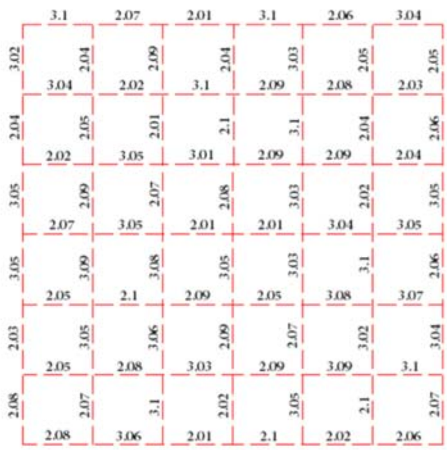
→ reptation algorithm





Shortest path

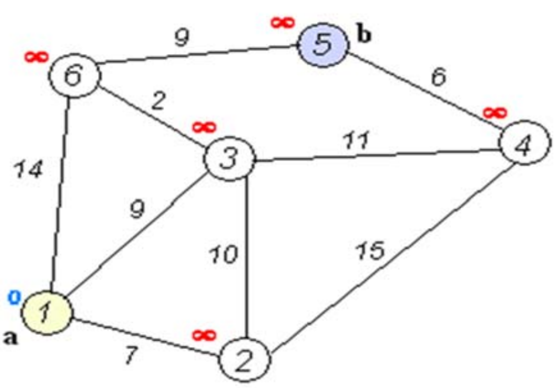
weighted graph

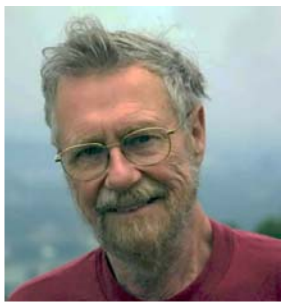


Dijkstra algorithm

greedy algorithm, i.e. tries to find a global optimum through many local optimizations.

(No greedy algorithm can solve travelling salesman problem.)





Edsger Dijkstra
1959

similar problem: minimum spanning tree

V. Jarník: *O jistém problému minimálním* [About a certain minimal problem], Práce Moravské Přírodovědecké Společnosti, 6, 1930, pp. 57–63. (in Czech)

Dijkstra algorithm

1. Assign to every node a tentative distance value: set it to zero for our initial node and to infinity for all other nodes.

2. Set the initial node as current. Mark all other nodes unvisited. Create a set of all the unvisited nodes called the *unvisited set*.

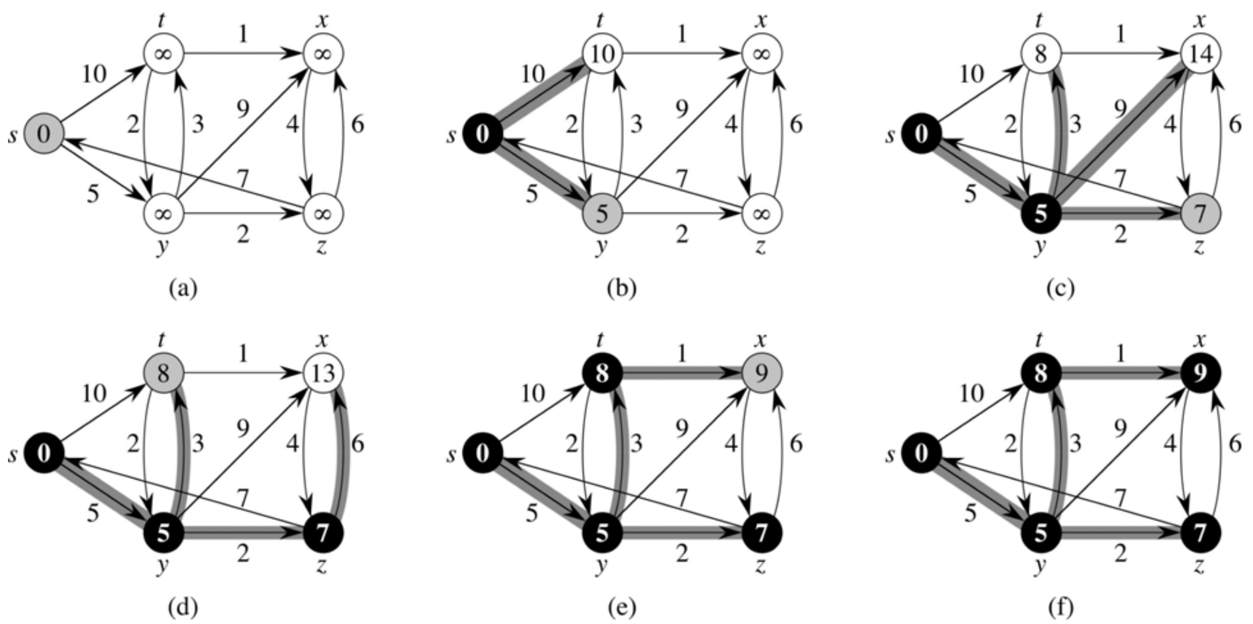
3. For the current node, consider all of its unvisited neighbors and calculate their *tentative* distances. Compare the newly calculated *tentative* distance to the current assigned value and assign the smaller one. For example, if the current node *A* is marked with a distance of 6, and the edge connecting it with a neighbor *B* has length 2, then the distance to *B* (through*A*) will be 6 + 2 = 8. If B was previously marked with a distance greater than 8 then change it to 8. Otherwise, keep the current value.

4. When we are done considering all of the neighbors of the current node, mark the current node as visited and remove it from the *unvisited set*. A visited node will never be checked again.

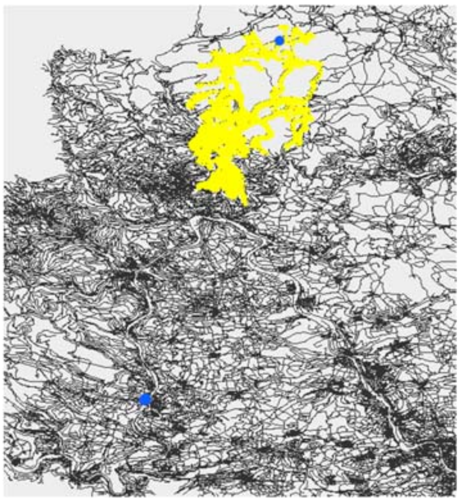
5. If the destination node has been marked visited (when planning a route between two specific nodes) or if the smallest tentative distance among the nodes in the *unvisited set* is infinity (when planning a complete traversal; occurs when there is no connection between the initial node and remaining unvisited nodes), then stop. The algorithm has finished.

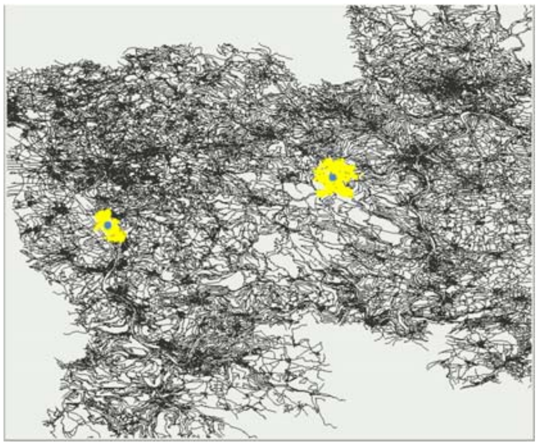
6. Otherwise, select the unvisited node that is marked with the smallest tentative distance, set it as the new "current node", and go back to step 3.

Dijkstra algorithm



Dijkstra algorithm





Bellman-Ford algorithm can also handle negative weights.

Simulated Annealing

- **P.J.M. Van Laarhoven and E.H. Aarts, „Simulated Annealing: Theory and Applications“ (Kluwer, 1987)**
- **A. Das and B.K. Chakrabarti (eds.), „Quantum Annealing and Related Optimization Methods“ Lecture Notes No. 679 (Springer, 1990)**

Simulated Annealing (SA)

ETH

S. Kirkpatrick, C.D. Gelatt and M.P. Vecci, 1983

SA is a stochastic optimization technique.

Given a finite set S of solutions

and a cost function F: $S \to \mathbb{R}$.

Search a global minimum:

$s^* \in S^* := \{ s \in S : F(s) \leq F(t) \;\; \forall\, t \in S \}$.

Difficult when S is very big (like $|S| = n!$).

Travelling Salesman

ETH

Given n cities σ_i and the travelling costs $c(\sigma_i, \sigma_j)$.

We search for the cheapest trip through all cities.

- $S = \{$ permutations of $\{1,..,n\} \}$
- $F(\sigma) = \Sigma_{i=1..n}\, c(\sigma_i, \sigma_j)$ für $\sigma \in S$

Finding the best trajectory is a NP-complete problem, i.e. time to solve grows faster than any polynomial of n.

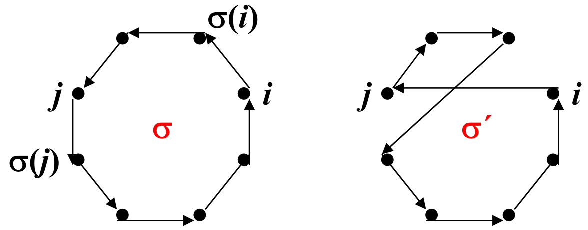
Travelling Salesman

Make local changes:

$\Rightarrow$ **Define closed configuration on S**

$N : S \rightarrow 2^S$ with $\sigma \in N(\sigma') \Leftrightarrow \sigma' \in N(\sigma)$

$\sigma' \in N(\sigma) \quad \Leftrightarrow$



Traditional optimization algorithm:

Improve systematically the costs by exploring close solutions.

If $F(\sigma') < F(\sigma)$ replace $\sigma := \sigma'$ until $F(\sigma) \leq F(t)$ for all $t \in N(\sigma)$.

Problem: One gets stuck in local minima.

Travelling Salesman

Simulated annealing optimization algorithm:

If $F(\sigma') \leq F(\sigma)$ replace $\sigma := \sigma'$

If $F(\sigma') > F(\sigma)$ replace $\sigma := \sigma'$

with probability $\exp(-\Delta F / T)$

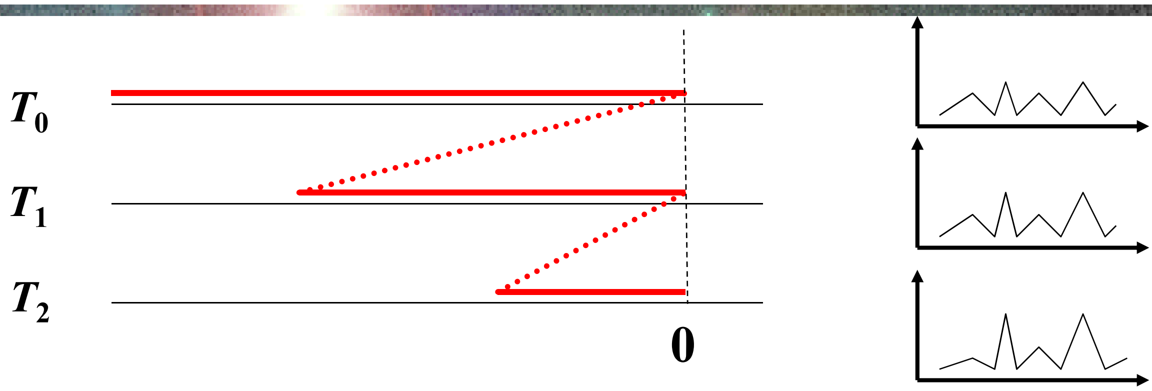
with $\Delta F = F(\sigma') - F(\sigma) > 0$

T is a constant (like a temperature)

Go slowly to $T \rightarrow 0$ in order to find global minimum.

Applet

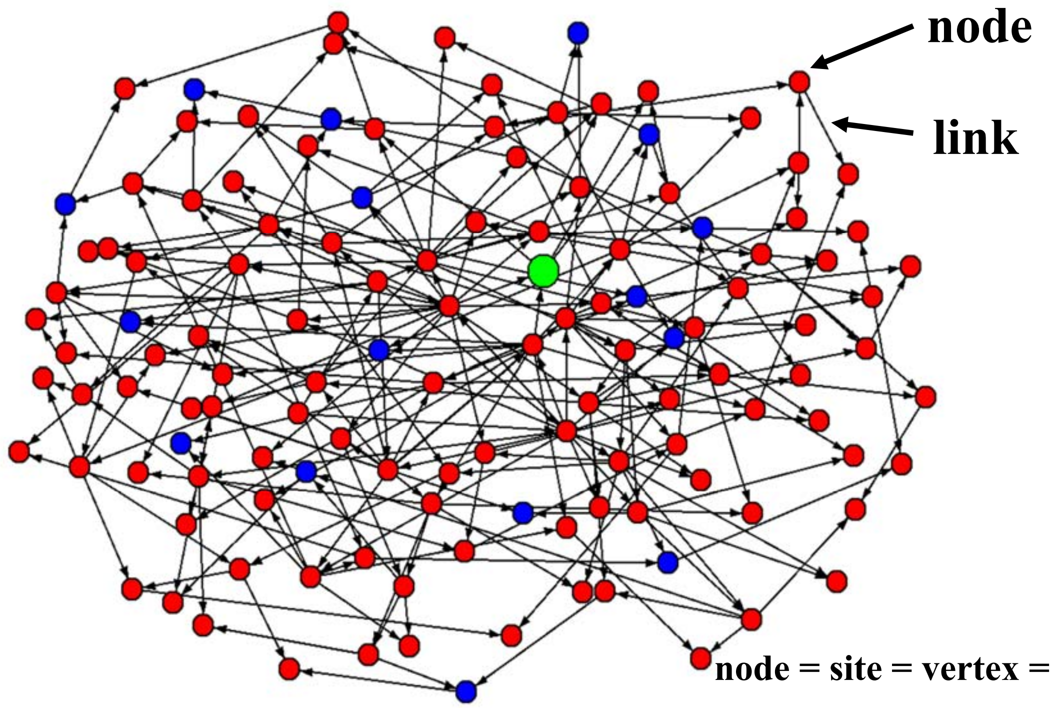
Slow cooling



Different cooling protocols are possible.

Asymptotic convergence is guarantied and leads to an exponential convergence time.

Complex networks



node = site = vertex = agent

link = bond = edge = connection

Complex Networks

- A.L. Barabasi: «Linked», Perseus, New York, 2003
- D.J. Watts: "Six Degrees", Norton, New York, 2003
- M. Buchanan: "Nexus", Norton, New York, 2003
- R. Pastor-Santorras and A. Vespigngani: "Evolution and Structure of the Internet", Cambridge Univ. Press, 2004
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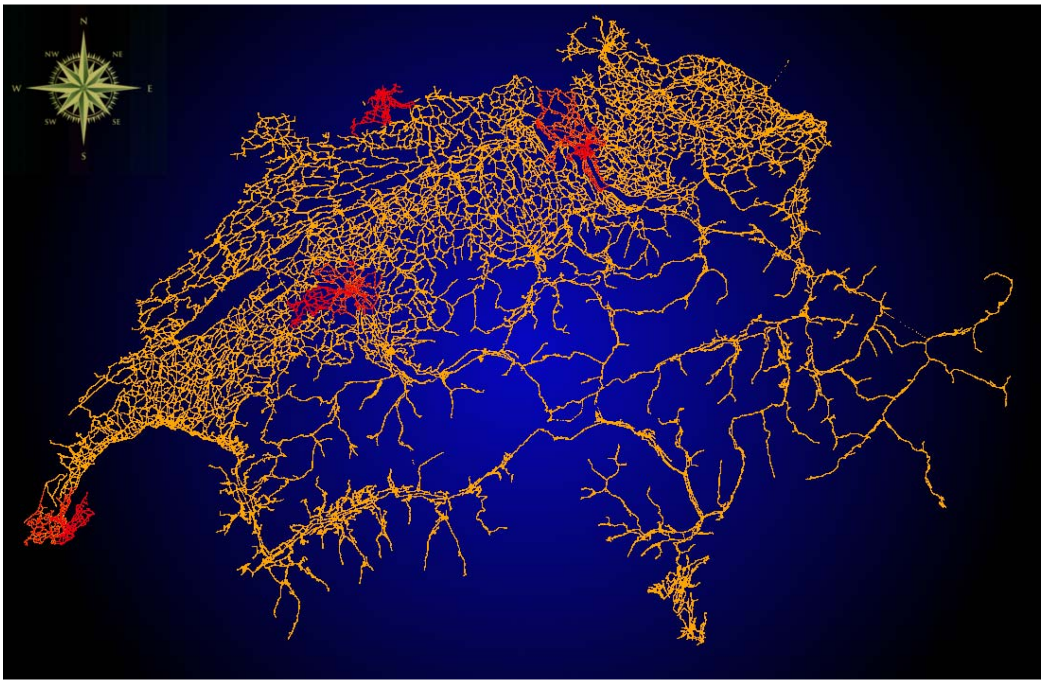
Technological Networks

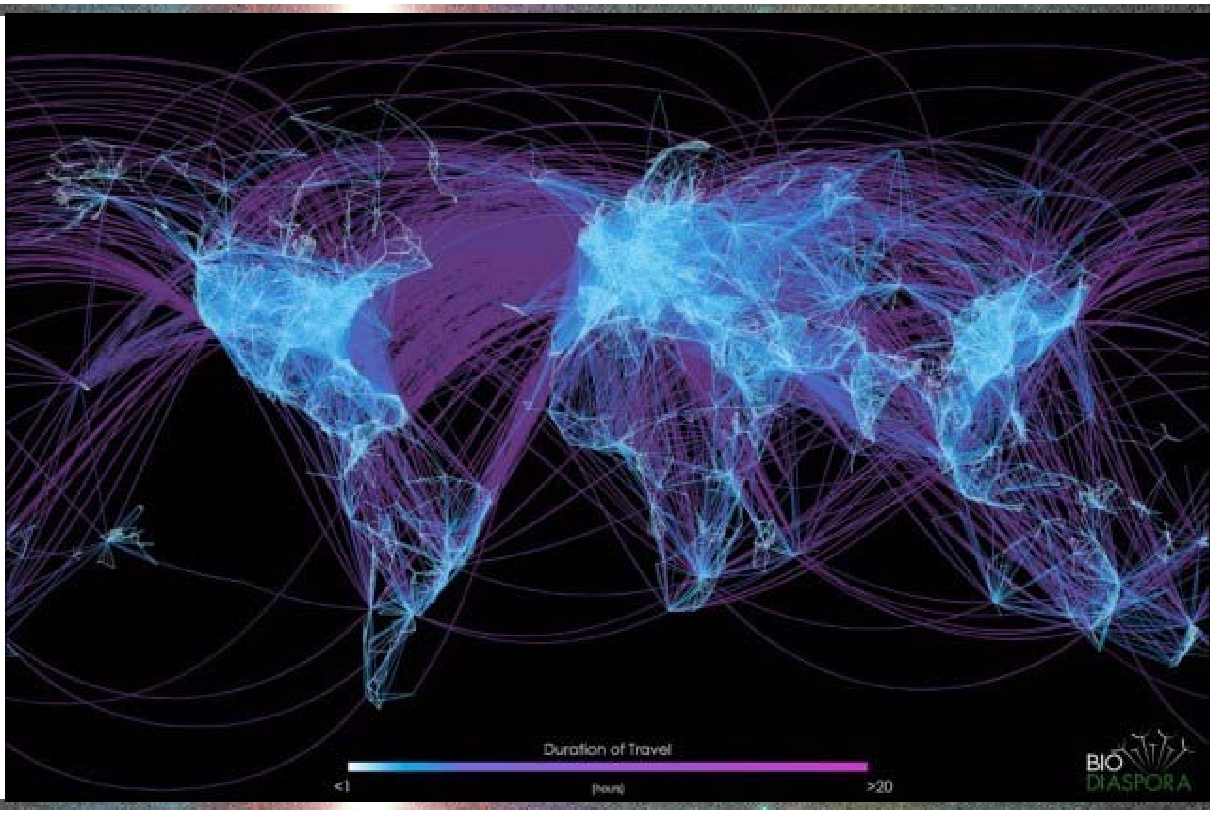
- Internet
- Railways
- Electrical grid
- Air traffic
- Gas pipes
- Highways
- WWW

Swiss roads

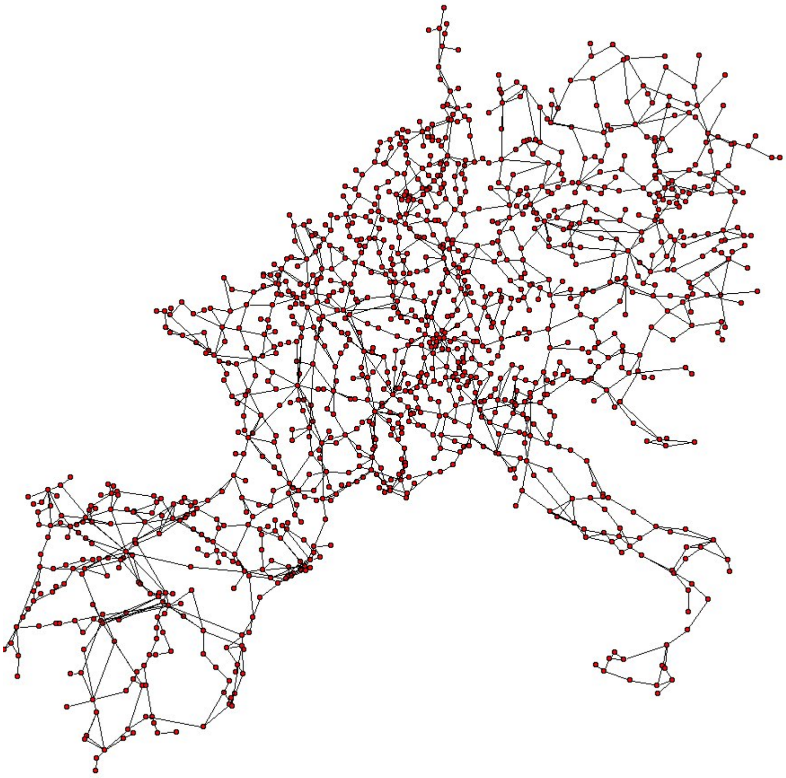


data from Helmut Honermann, Bundesamt für Raumentwicklung, ARE

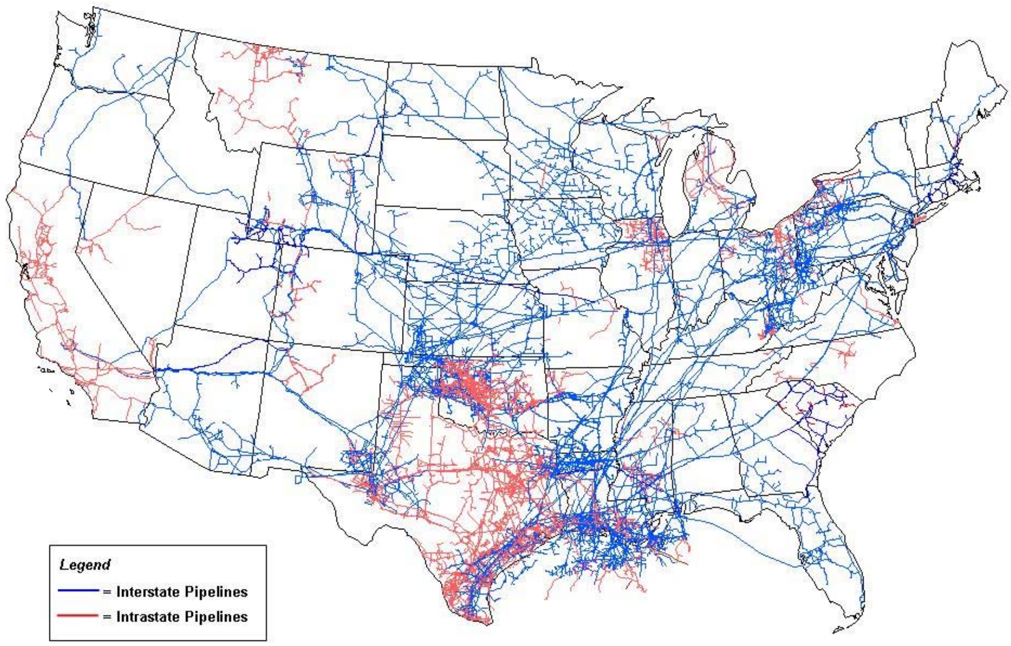
World Airline Network (WAN)



European Power Grid

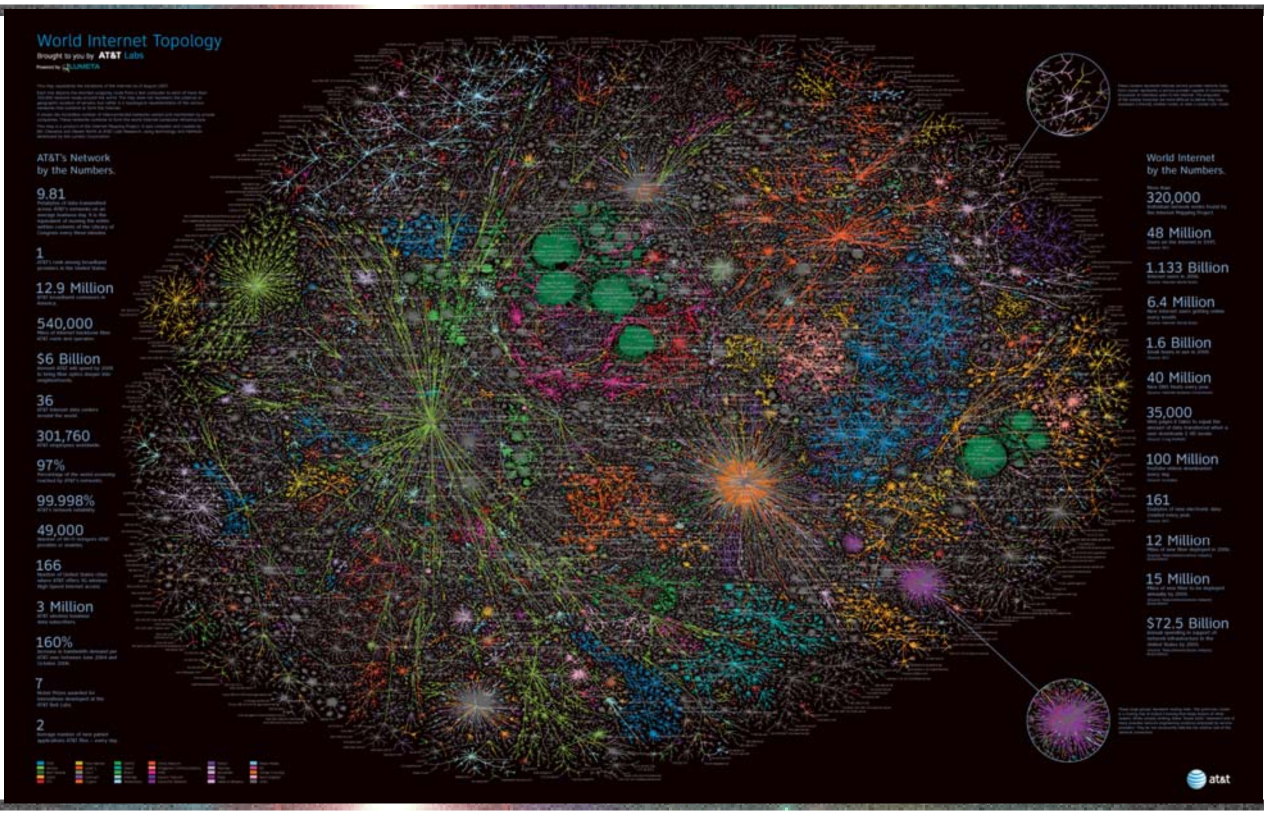


Natural gas pipeline network



Source: Energy Information Administration, Office of Oil & Gas, Natural Gas Division, Gas Transportation Information System

The Internet

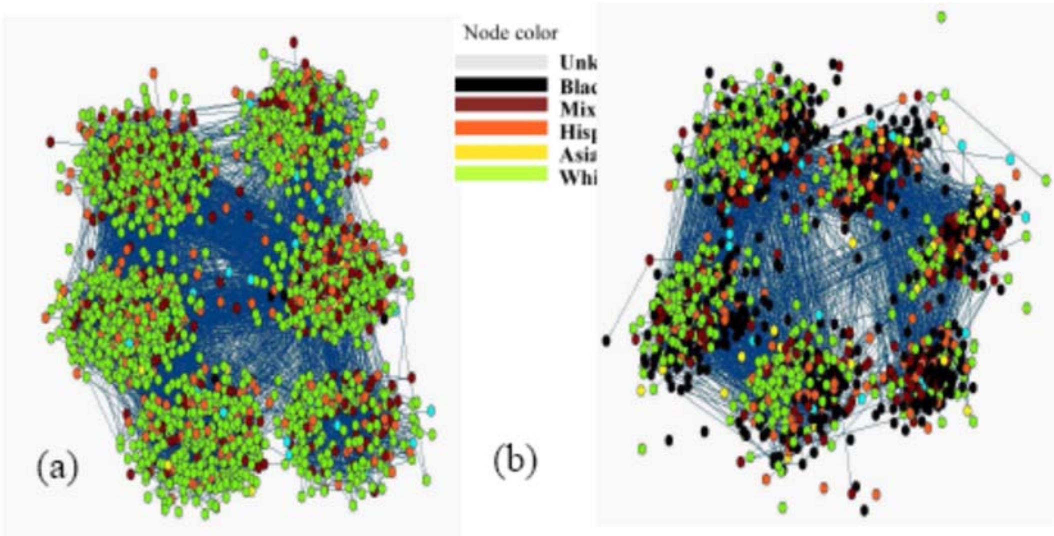


Social Networks

- Friendships
- Sexual relations
- Collaborations
- Criminal associations
- Financial institutions
- Gossip
- Elections
- Spam

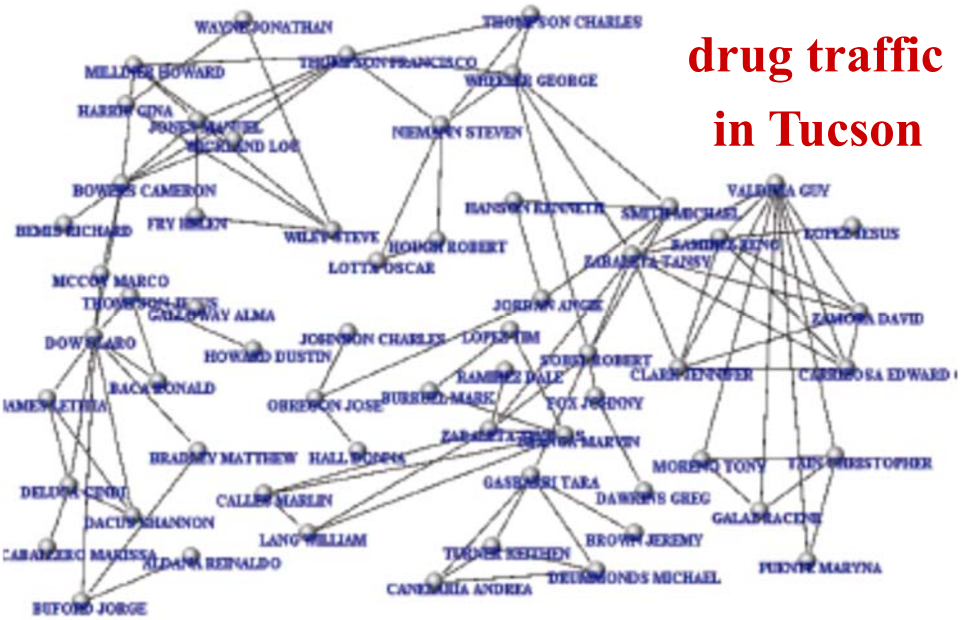
Friendships in schools

Survey interviewing 90118 student from 84 schools in US
(Add Health Program)



visualization using „pajec“

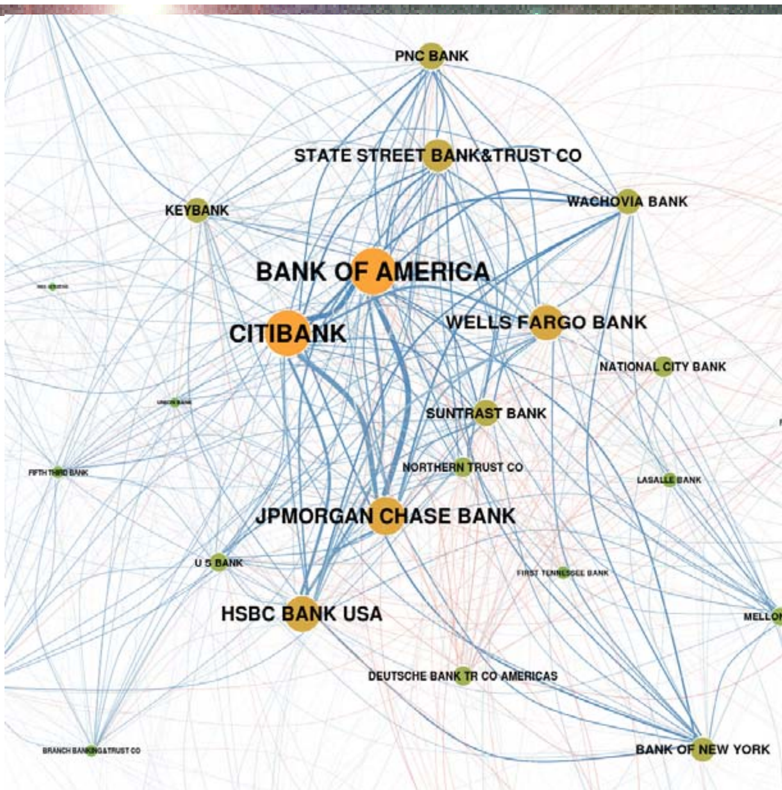
Criminal network



drug traffic
in Tucson

Social Network Analysis (SNA) from Anacapa

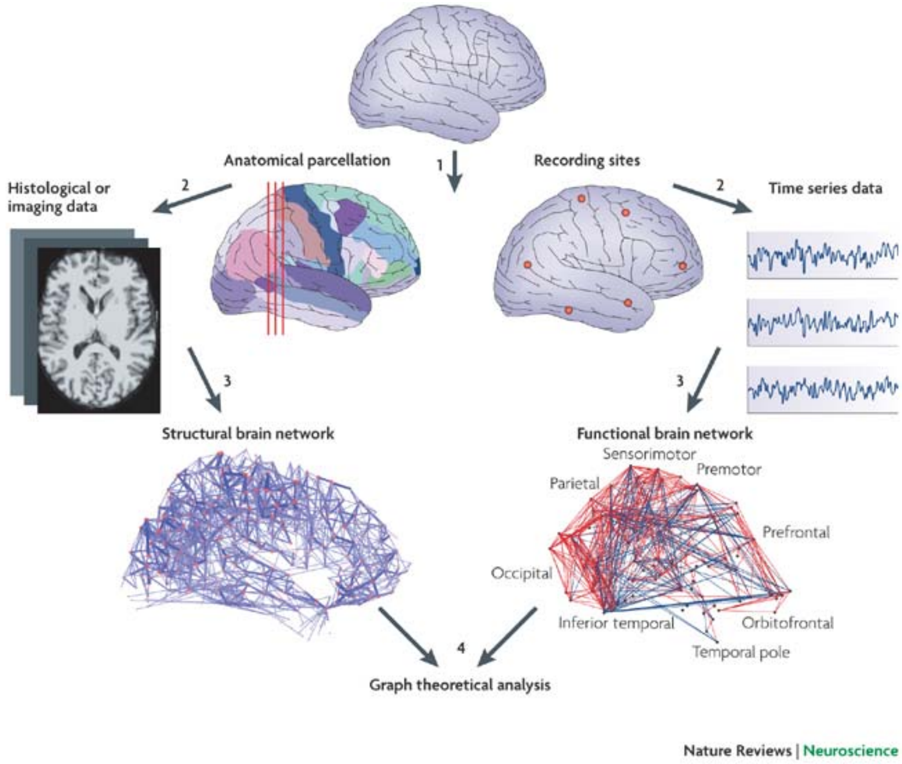
Financial institutions



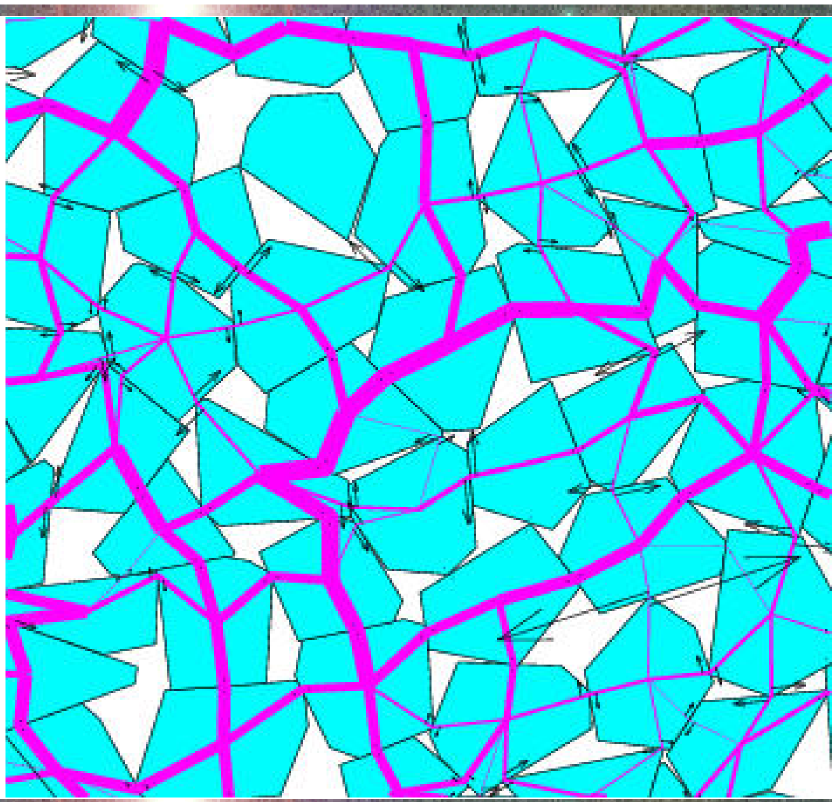
Natural Networks

- Brain
- Gels
- Contact networks
- Rivers
- Colloidal Structures
- Protein networks
- Food Webs

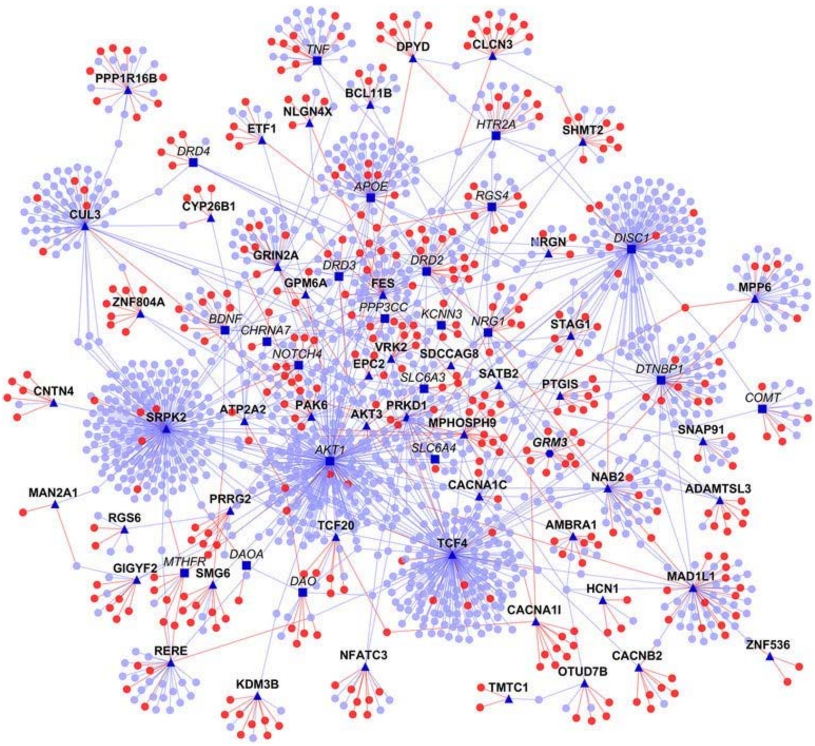
Brain



Contact Network



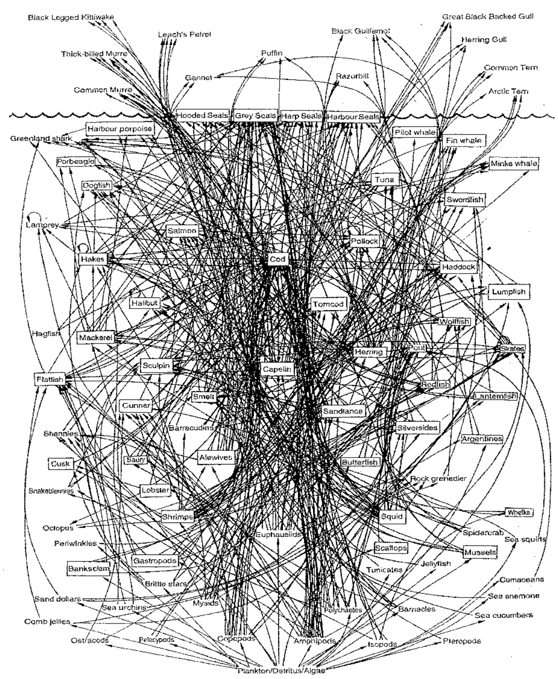
Protein interaction network



Protein-protein interaction for schizophrenia associated proteins

Interaction between protein can be defined by how closely located on a DNA are the genes that encode the two proteins.

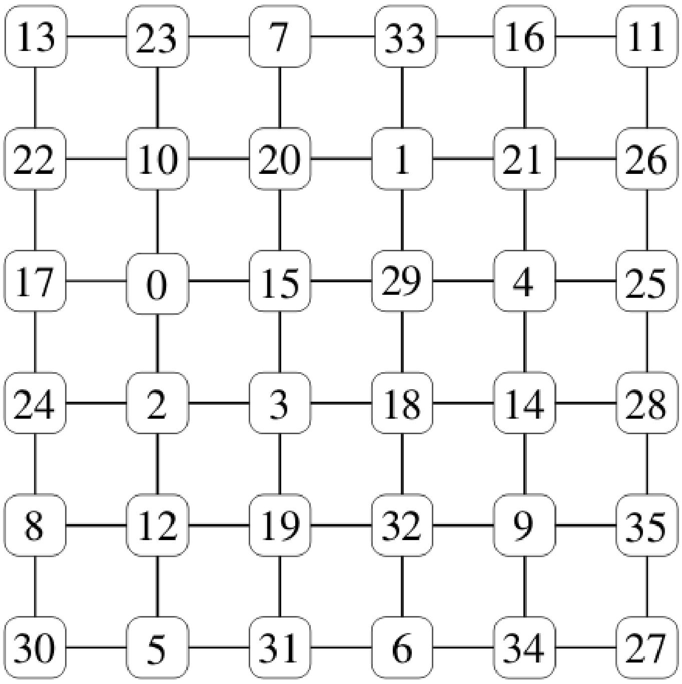
Food Chain Network



Food web of the North Atlantic Ocean

predator → prey

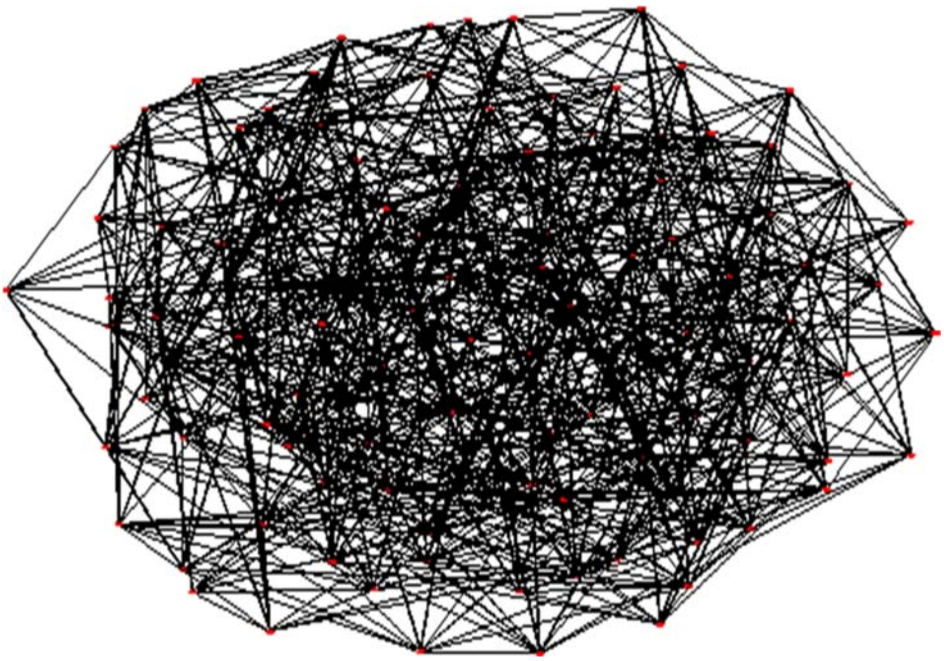
Simplest Network



square lattice

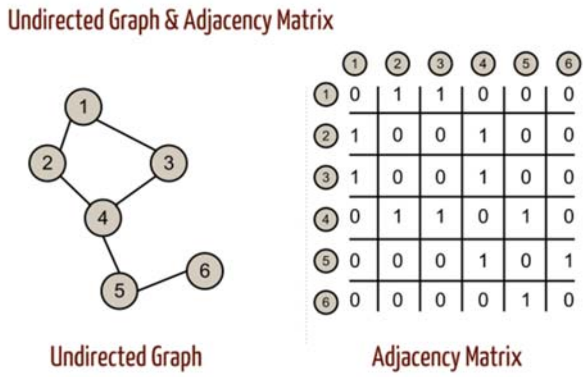
each agent has a unique index

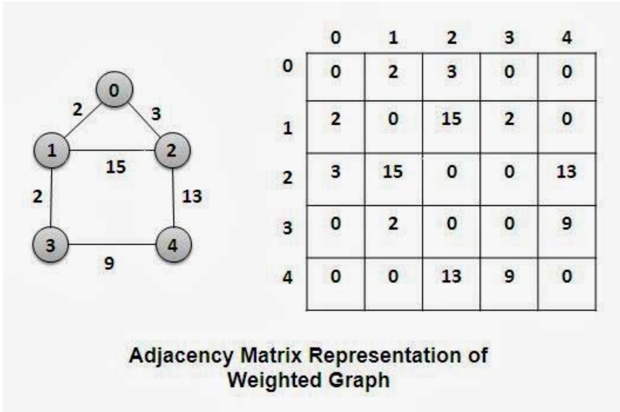
Erdös – Rényi (ER)

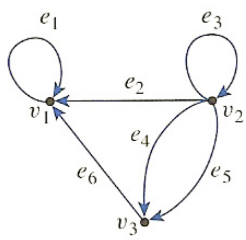


Every pair of nodes is connected.

Adjacency Matrix



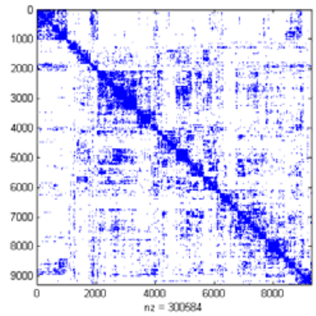




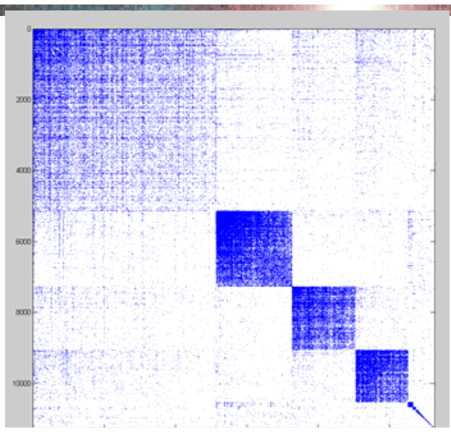
Directed Graph G

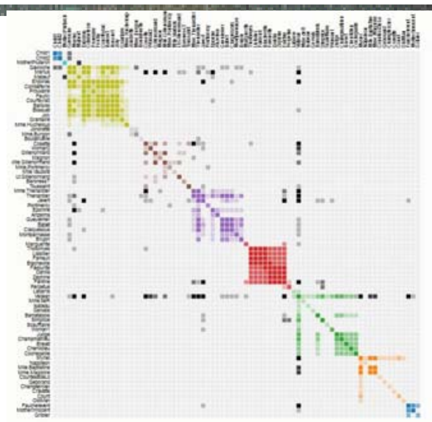
$$\mathbf{A} = \begin{array}{c} \\ v_1 \\ v_2 \\ v_3 \end{array} \begin{array}{c} \begin{array}{ccc} v_1 & v_2 & v_3 \end{array} \\ \begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 2 \\ 1 & 0 & 0 \end{bmatrix} \end{array}$$

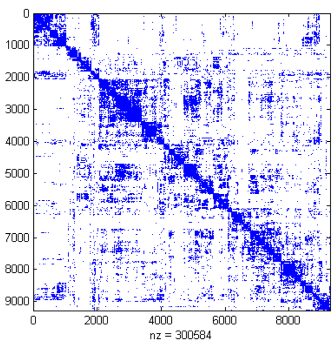
Adjacency Matrix

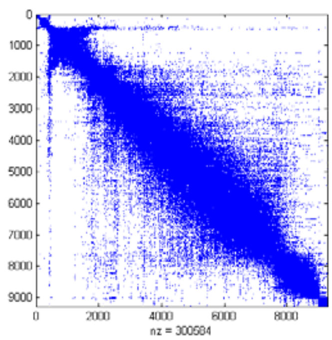


Adjacency Matrix









Complex Structures of Networks

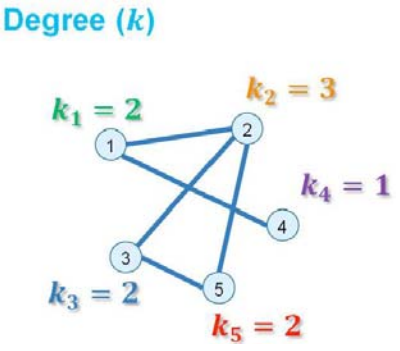
- Scale-free
- Small world
- Modular

Properties of networks

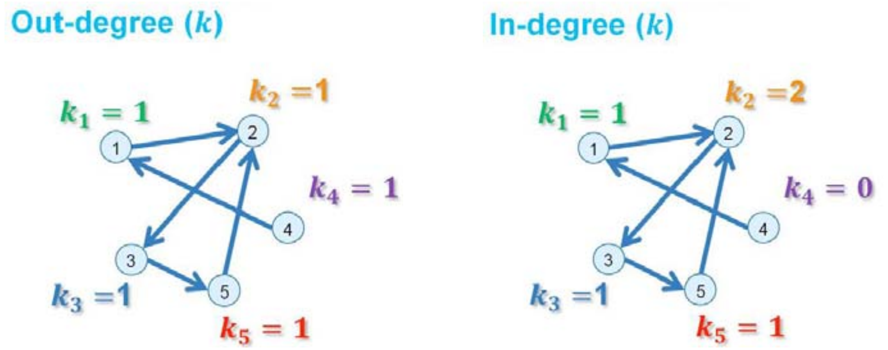
- Degree distribution
- Clustering Coefficient
- Shortest Path
- Assortativity
- Betweenness Centrality
- Cliquishness
- Connectivity Correlation
- Cutting bonds, bottlenecks
- ……

Degree

degree k is the number of connections of a site



directed networks:



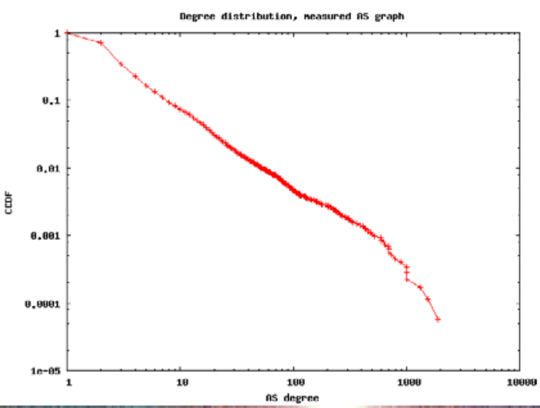
Scale-free networks

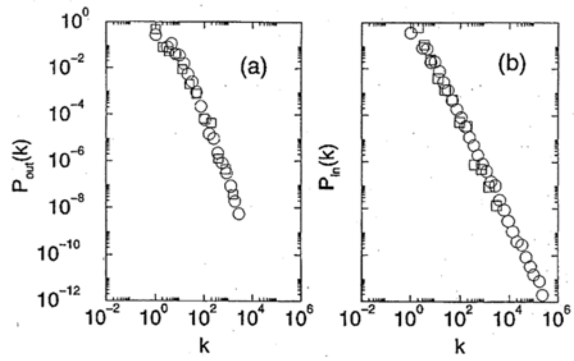
degree k is the number of connections of a site

A network is called «scale-free» if its distribution of degrees follows:

$$\boxed{P(k) \propto k^{-\gamma}}$$

internet: $\boxed{\gamma = 2.4}$ **www:** $\boxed{\gamma_{out} = 2.4}$ $\boxed{\gamma_{in} = 2.1}$

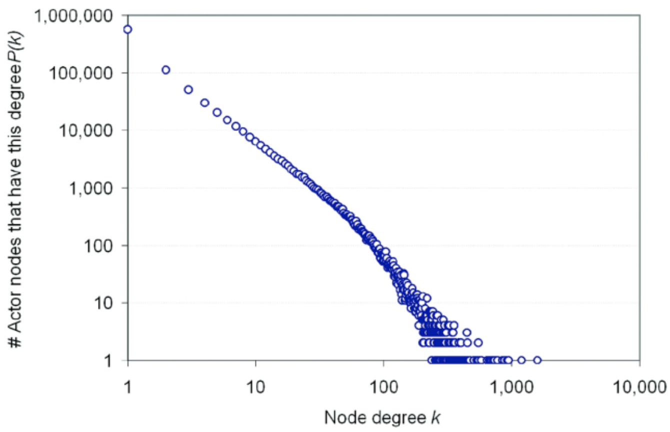




Scale-free networks

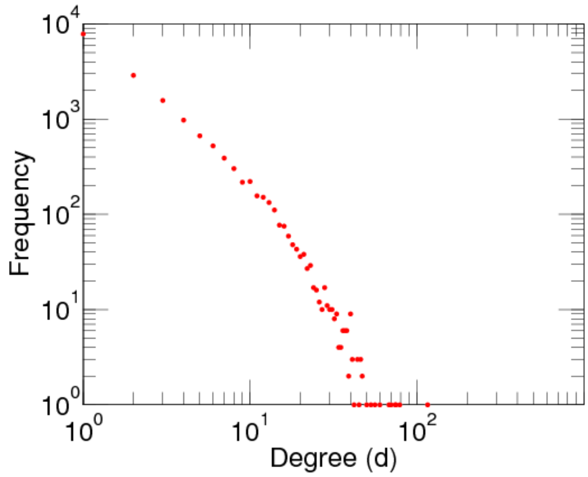
collaborations

movie actors: $\boxed{\gamma = 2.3}$



scientific collaborations:

(bipartite network of authors and papers taken from arXiv cond-mat)



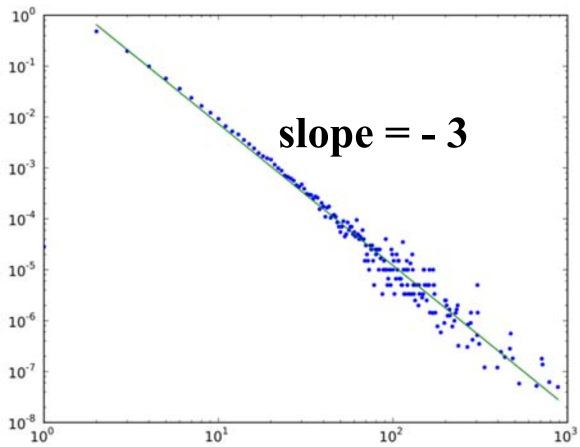
Scale-free networks

Barabasi-Albert model: (1998)

preferential attachment:

attach new sites to a site of degree k with probability proportional to k

$\rightarrow \gamma = 3$



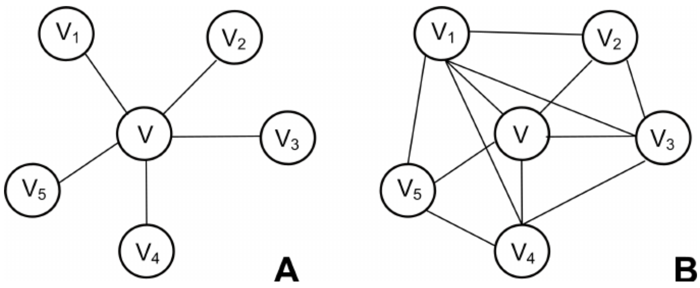
„configuration model“:

attach new sites to a site of degree k with probability proportional to $k^{-\alpha}$

Small-world property

clustering coefficient

$C = \frac{2}{k(k-1)} \times$ number of connections between neighbors



shortest path

$l = \langle$ chemical distance between two sites $\rangle$

Stanley Milgram

«six degrees of separation»

Duncan Watts

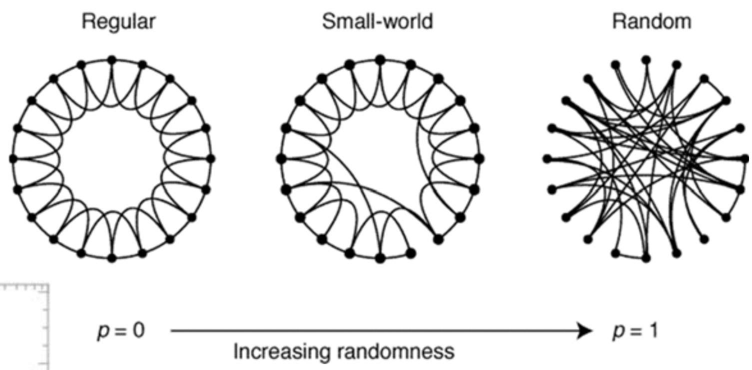
Steven Strogatz

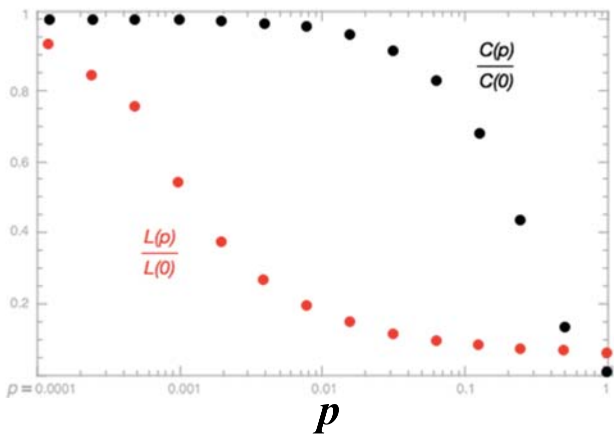
A network has «small-world property», when $0.5 < C \leq 1$ and l does not grow faster than $\log N$.

Small-world property

D.J. Watts and S.H. Strogatz, Nature, 1998

Start with regular lattice with degree k and rewire a fraction p of its connections.





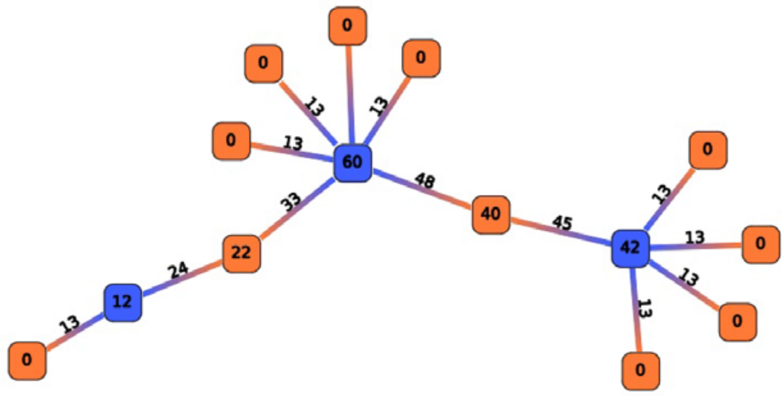
$$C(p=0) = \frac{3(k-2)}{4(k-1)}$$

$$l(p=1) = \frac{\ln N}{\ln k}$$

Betweeness centrality

$$g(v) = \frac{2}{(N-1)(N-2)} \sum_{i,j\neq v} \frac{\text{number of shortest paths from } i \text{ to } j \text{ through } v}{\text{number of shortest paths from } i \text{ to } j}$$

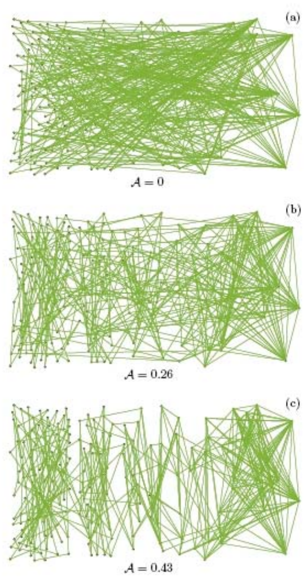
Measures the load during traffic.



Assortativity

The assortativity A describes the correlation between the degree of the nodes at each side of an edge:

$$\boxed{A = \frac{4M\sum_i j_i k_i - \left(\sum_i (j_i + k_i)\right)^2}{2M\sum_i \left(j_i^2 + k_i^2\right) - \left(\sum_i (j_i + k_i)\right)^2}}$$

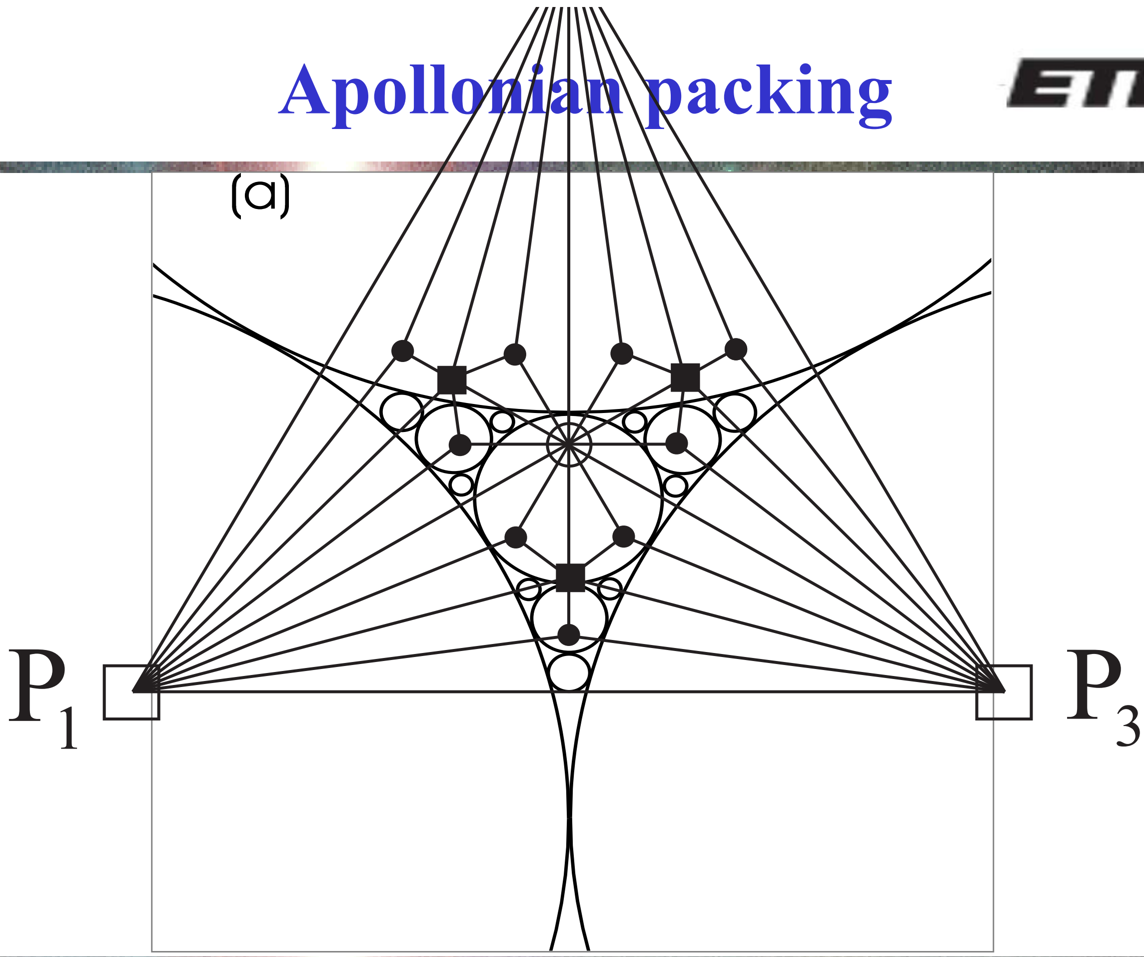


where M is the number of edges and j_i and k_i the degrees of the nodes connected by the edge i. The range of A is between -1 and 1. A positive value indicates that nodes with similar degrees are connected, while a negative value indicates that nodes with low degree are attached to nodes with high degree and vice versa.

Questions

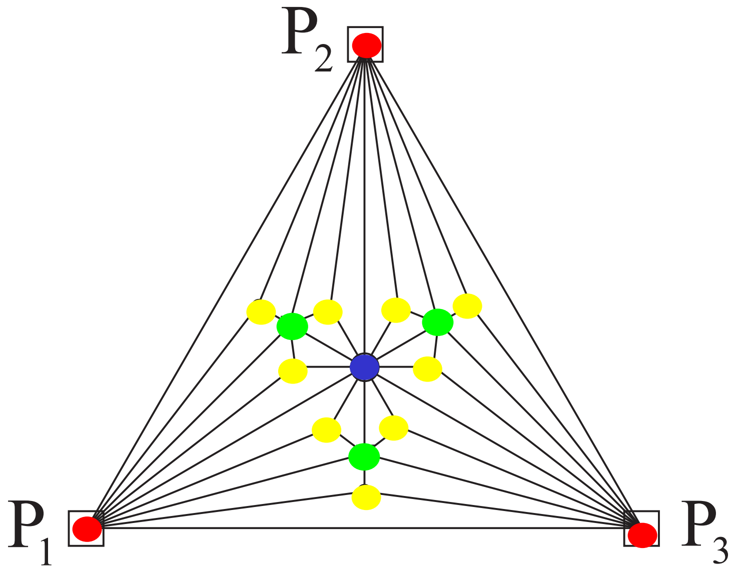
- Propagation of information or epidemics
- Robustness against attack
- Synchronization of oscillators
- Clogging, gridlock of traffic
- Basins of attraction, cycles
- Optimization dynamics
- Self-repair, complementation

Apollonian packing



Apollonian network

- scale-free
- small world
- Euclidean
- space-filling
- matching



Applications

- Systems of electrical supply lines
- Friendship networks
- Computer networks
- Force networks in polydisperse packings
- Highly fractured porous media
- Networks of roads

Degree distribution

scale-free: $P(k) \propto k^{-\gamma}$

$\Rightarrow \quad W(k) \propto k^{1-\gamma}$

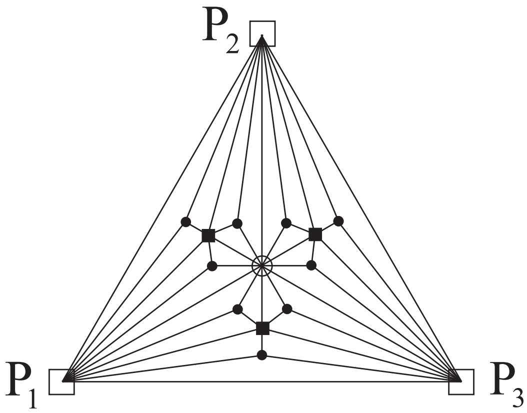
$m(k,n)$	k
3^n	3
3^{n-1}	3×2
3^{n-2}	3×2^2
$\vdots$	$\vdots$
3^2	$3 \times 2^{n-1}$
3	3×2^n
1	2^{n+1}

$$\Rightarrow \gamma - 1 = \frac{\ln 3}{\ln 2} \approx 1.585$$

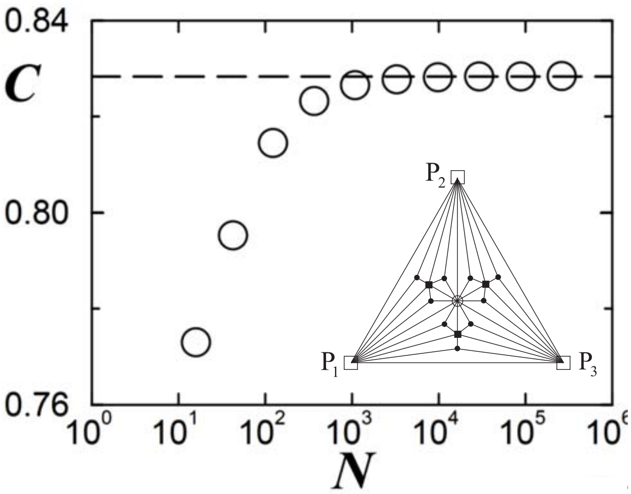
$N_n =$ number of sites at generation n

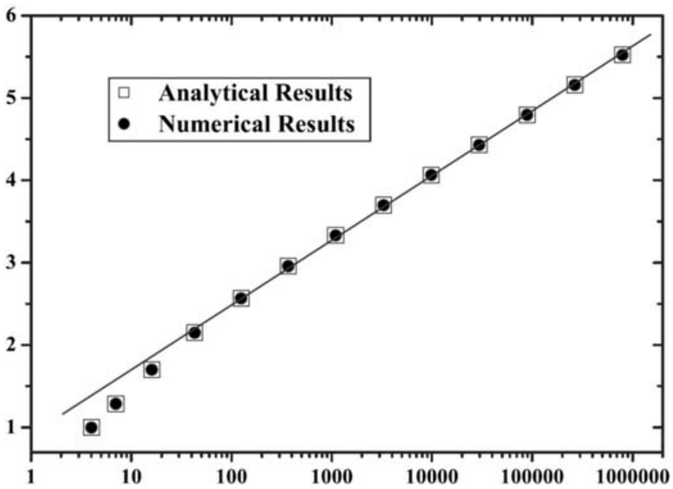
$m(k,n) =$ number of vertices of degree k

cummulative distribution $W(k) = \sum_{k'>k} m(k',n) / N_n$



Small-world properties





clustering coefficient

$$C = \frac{2}{k(k-1)} \times \text{number of connections between neighbors}$$

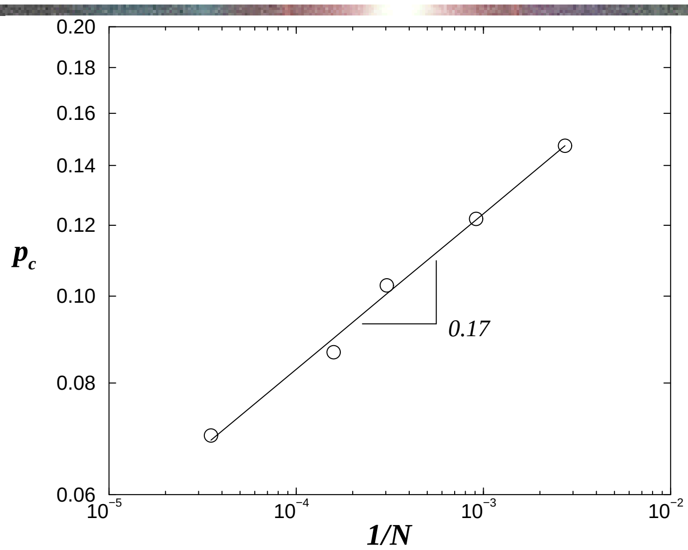
$$\boxed{C = 0.828}$$

shortest path

$$l = \langle \text{chemical distance between two sites} \rangle$$

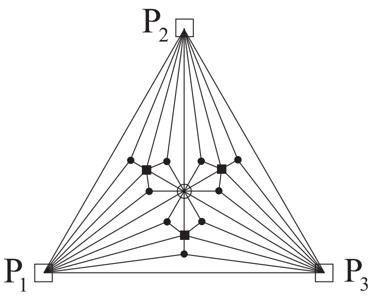
$$\boxed{l \propto \ln N}$$

Percolation threshold



epidemics

random failure



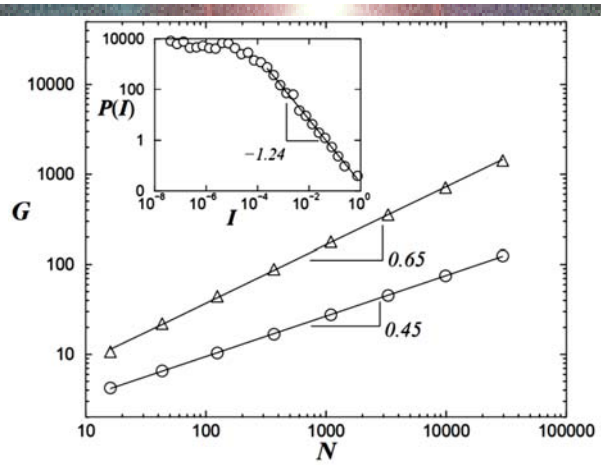
bond percolation

at p_c : P_1, P_2 and P_3 simultaneously connected

$$p_c \propto L^{-\frac{1}{\nu}}, L = \sqrt{N} \Rightarrow \nu \approx 3$$

porous media $\Rightarrow$ Archie's law

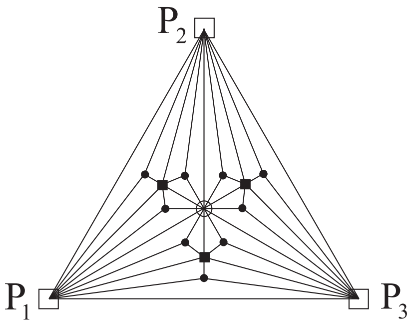
Electrical conductance



flux

fuses =

malicious attack



- from center to all sites of generation n:

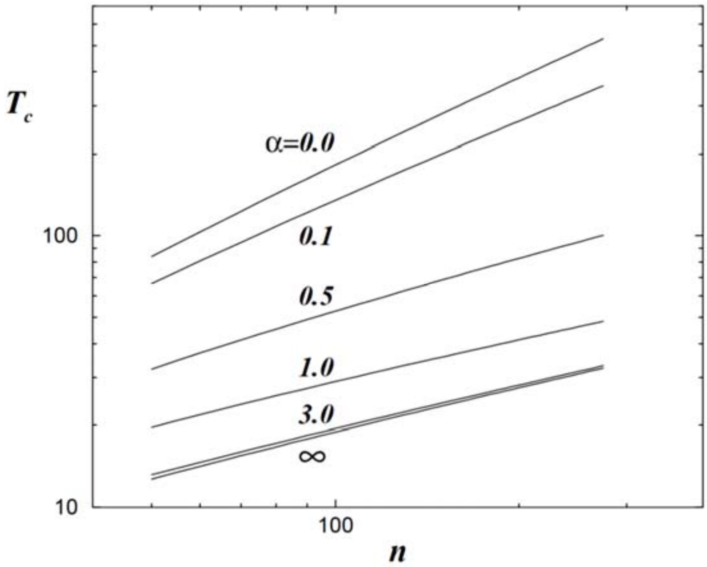
$$\left.\begin{matrix} S_1 \\ S_2 \end{matrix}\right\} = \text{number of outputs of } \left\{\begin{matrix} \text{system} \\ \text{each site} \end{matrix}\right.$$

$$n-1 \rightarrow n \Rightarrow S_1 \rightarrow 3 * S_1, S_2 \rightarrow 2 * S_2 \quad \Rightarrow \quad z = 2/3$$

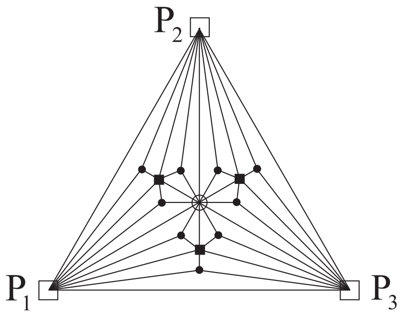
current distribution $P(I) \propto I^{-1.24}$

- from P_1 to P_2 : $z \approx 0.45$

Ising model



opinion



coupling constant $J_n \propto n^{-\alpha}$

correlation length J_n diverges at T_c

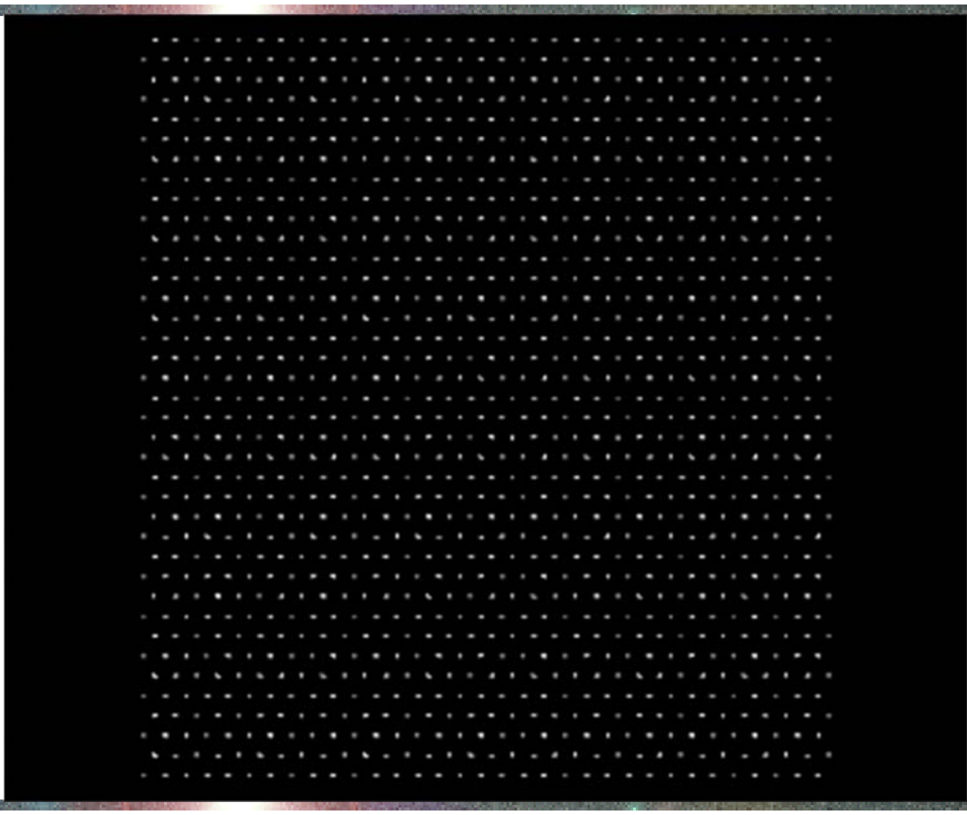
free energy, entropy, specific heat are smooth

magnetization $m \propto e^{-T^{\lambda}}$ $T \to \infty$

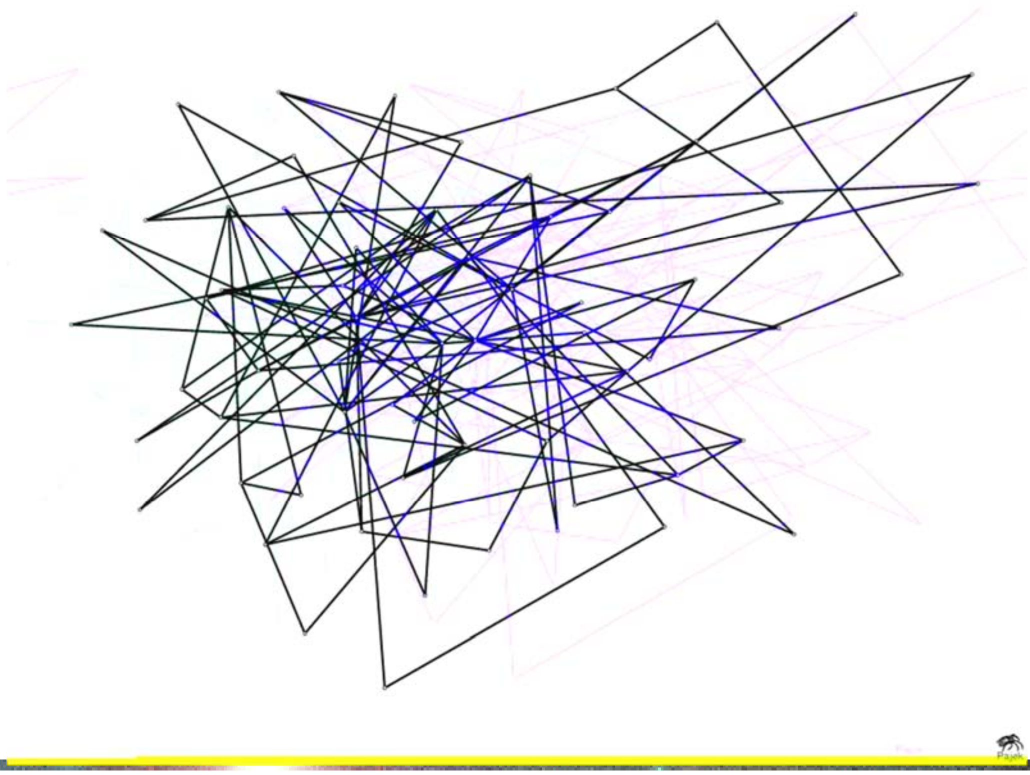
Apollonian networks

- Extremely stable against random failure.
- Very fragile against malicious attacks.
- Only one opinion

Evolution of epidemics with healing on a mobile population



Optimizing through rewiring



Numerical Methods

Solving equations

Finding the solution (root) of an equation:

$$f(x) = 0$$

is equivalent to the optimization problem of finding the minimum (or maximum) of $F(x)$ given by:

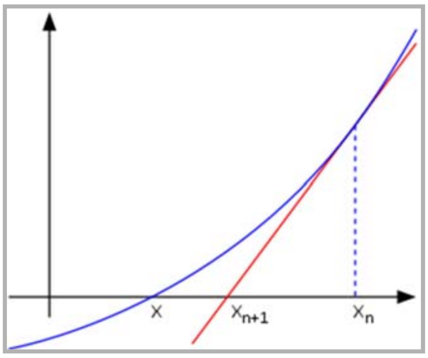
$$\boxed{\frac{d}{dx} F(x) = 0}$$

Newton method

Be x_0 a first guess, then linearize around x_0:

$$\boxed{f(x_1) \approx f(x_0) + (x_1 - x_0) f'(x_0) = 0}$$

$$\boxed{x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}}$$



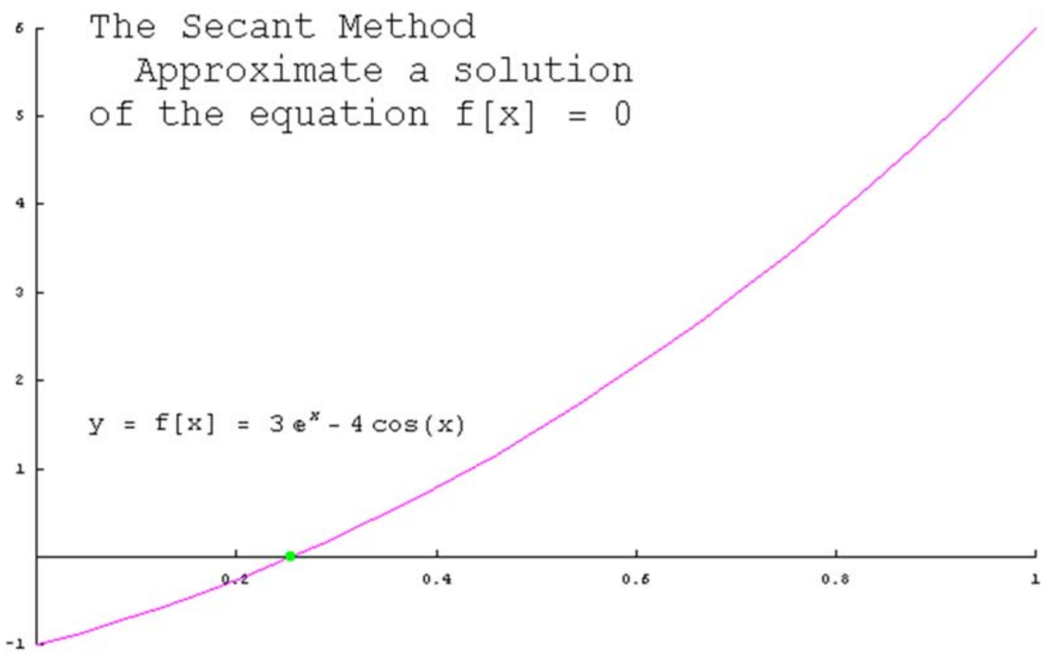
Secant method

If derivative of f is not known analytically:

$$\boxed{f'(x_n) \approx \frac{f(x_n) - f(x_{n-1})}{x_n - x_{n-1}}}$$

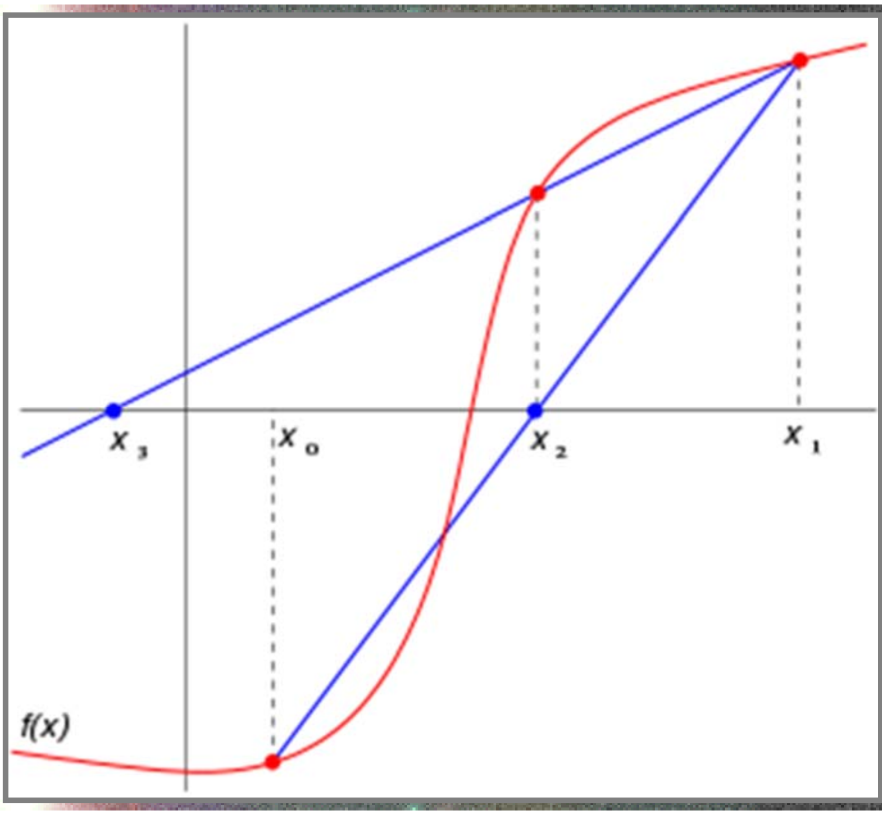
$$\boxed{x_{n+1} = x_n - (x_n - x_{n-1}) \frac{f(x_n)}{f(x_n) - f(x_{n-1})}}$$

Secant method



Secant method

Might not converge



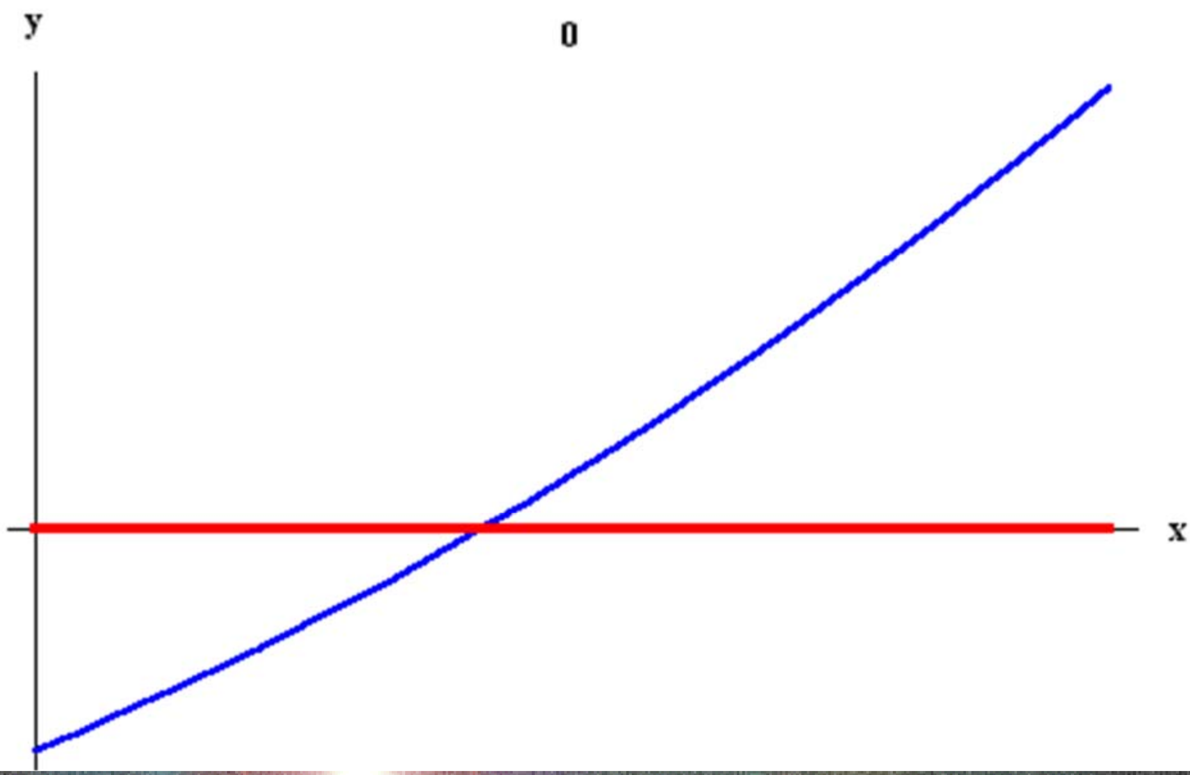
Bisection method

Take two starting values x_1 and x_2 with $f(x_1) < 0$ and $f(x_2) > 0$.

Define mid-point x_m as $x_m = (x_1 + x_2) / 2$.

If $\mathrm{sign}(f(x_m)) = \mathrm{sign}(f(x_1))$
then replace x_1 by x_m
otherwise replace x_2 by x_m.

Bisection method



Regula falsi

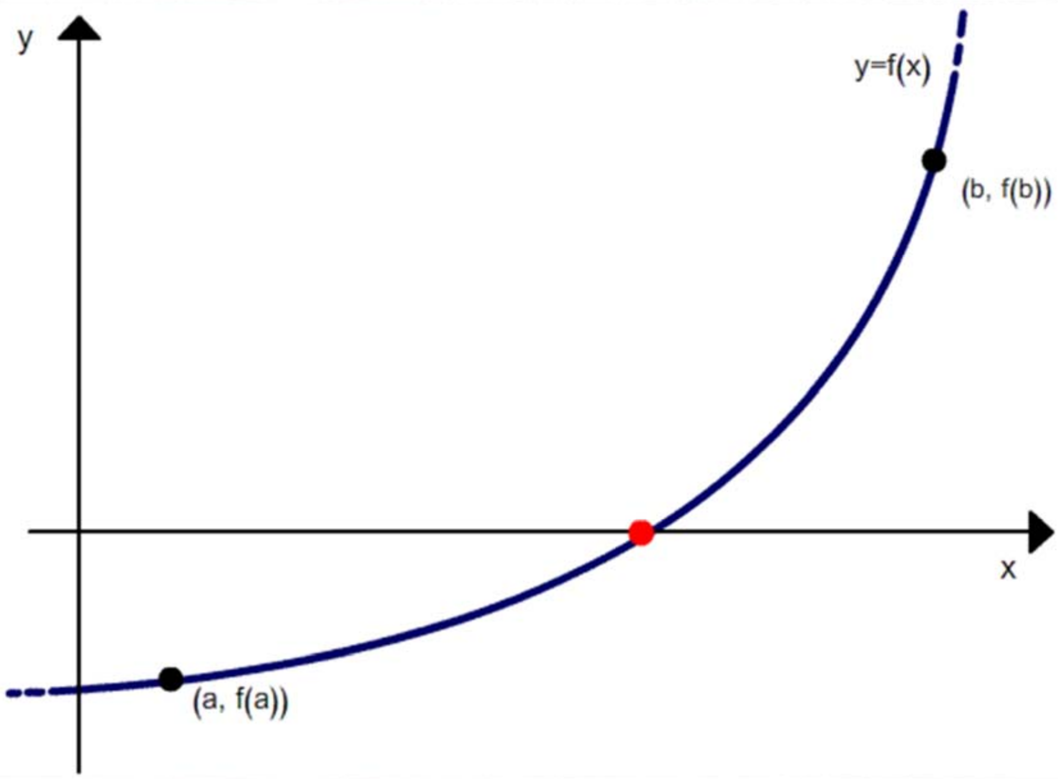
Take two starting values x_1 and x_2 with $f(x_1) < 0$ and $f(x_2) > 0$.

Approximate f by a straight line between $f(x_1)$ and $f(x_2)$ and calculate its root as:

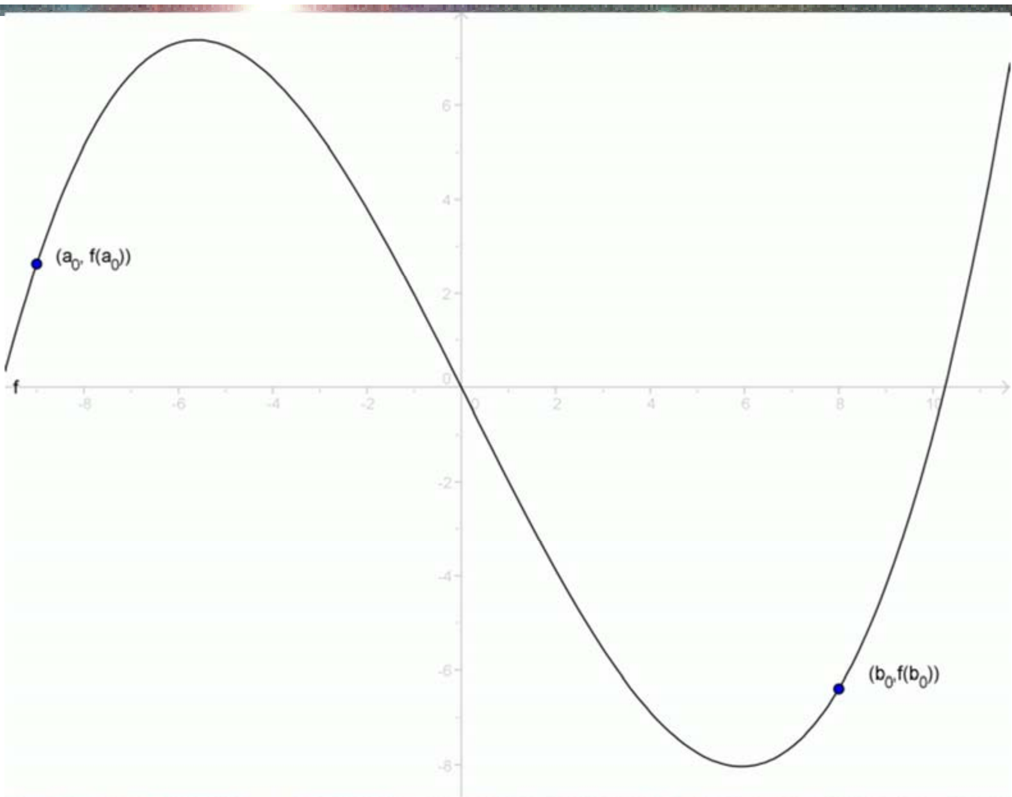
$$x_m = (f(x_1)\,x_2 - f(x_2)\,x_1) \,/\, (f(x_1) - f(x_2)).$$

If $\mathrm{sign}(f(x_m)) = \mathrm{sign}(f(x_1))$, then replace x_1 by x_m otherwise replace x_2 by x_m.

Regula falsi



Regula falsi



N-dimensional equations

Be $\vec{x}$ a *N*-dimensional vector.

System of *N* coupled equations:

$$\boxed{\vec{f}(\vec{x}) = 0}$$

corresponding to the *N*-dimensional optimization problem:

$$\boxed{\vec{\nabla} F(\vec{x}) = 0}$$

N-dimensional Newton method

Define the Jacobi matrix:

$$\boxed{J_{i,j}(\vec{x}) = \frac{\partial f_i(\vec{x})}{\partial x_j}}$$

Must be non-singular and also well-conditioned for numerical inversion.

$$\boxed{\vec{x}_{n+1} = \vec{x}_n - \overleftrightarrow{J}^{-1}\vec{f}(\vec{x}_n)}$$

System of linear equations

$$\begin{array}{l} b_{11}x_1 + \ldots + b_{1N}x_N = c_1 \\ \vdots \\ b_{N1}x_1 + \ldots + b_{NN}x_N = c_N \end{array} \iff \overleftrightarrow{B}\vec{x} = \vec{c}$$

solution: $\boxed{\vec{x} = \overleftrightarrow{B}^{-1}\vec{c}}$

System of linear equations

$$\boxed{\vec{f}(\vec{x}) = \overleftrightarrow{B}\vec{x} - \vec{c} = 0 \Rightarrow \overleftrightarrow{J} = \frac{\partial f_i(\vec{x})}{\partial x_j} = \overleftrightarrow{B}}$$

apply Newton method: $\boxed{\vec{x}_{n+1} = \vec{x}_n - \overleftrightarrow{J}^{-1}\vec{f}(\vec{x}_n)}$

$$\boxed{\vec{x}_{n+1} = \vec{x}_n - \overleftrightarrow{B}^{-1}(\overleftrightarrow{B}\vec{x}_n - \vec{c}) = \overleftrightarrow{B}^{-1}\vec{c}}$$

$\Rightarrow$ **exact solution in one step**

N-dimensional secant method

If the derivatives are not known analytically:

$$\boxed{J_{i,j}(\vec{x}) = \frac{f_i(\vec{x} + h_j\vec{e}_j) - f_i(\vec{x})}{h_j}}$$

where h_j should be chosen as:

$$\boxed{h_j \approx x_j\sqrt{\varepsilon}}$$

being ε the machine precision,
i.e. $\approx 10^{-16}$ for a 64 bit computer.

Other techniques

Relaxation method:

$$\boxed{\vec{f}(\vec{x}) = 0 \quad \rightarrow \quad x_i = g_i(x_j, j \neq i), \quad i = 1, \ldots, N}$$

Start with $x_i(0)$ and iterate: $x_i(t+1) = g_i(x_j(t))$.

Gradient methods:

1. Steepest descent
2. Conjugate gradient

Ordinary differential equations

First order ODE, initial value problem:

$$\boxed{\frac{dy}{dt} = f(y,t)}$$ with $y(t_0) = y_0$

examples:

radioactive decay $\boxed{\frac{dN}{dt} = -\lambda N}$

coffee cooling $\boxed{\frac{dT}{dt} = -\gamma(T - T_{room})}$

Euler method

explicit forward integration algorithm

choose small Δt, Taylor expansion:

$$y(t_0+\Delta t) = y(t_0) + \Delta t \frac{dy}{dt}(t_0) + O(\Delta^2 t)$$
$$= y_0 + \Delta t \cdot f(y_0, t_0) + O(\Delta^2 t) \equiv y(t_1) \equiv y_1$$

convention: $t_n = t_0 + n\Delta t \ , \quad y_n = y(t_n)$

Euler method

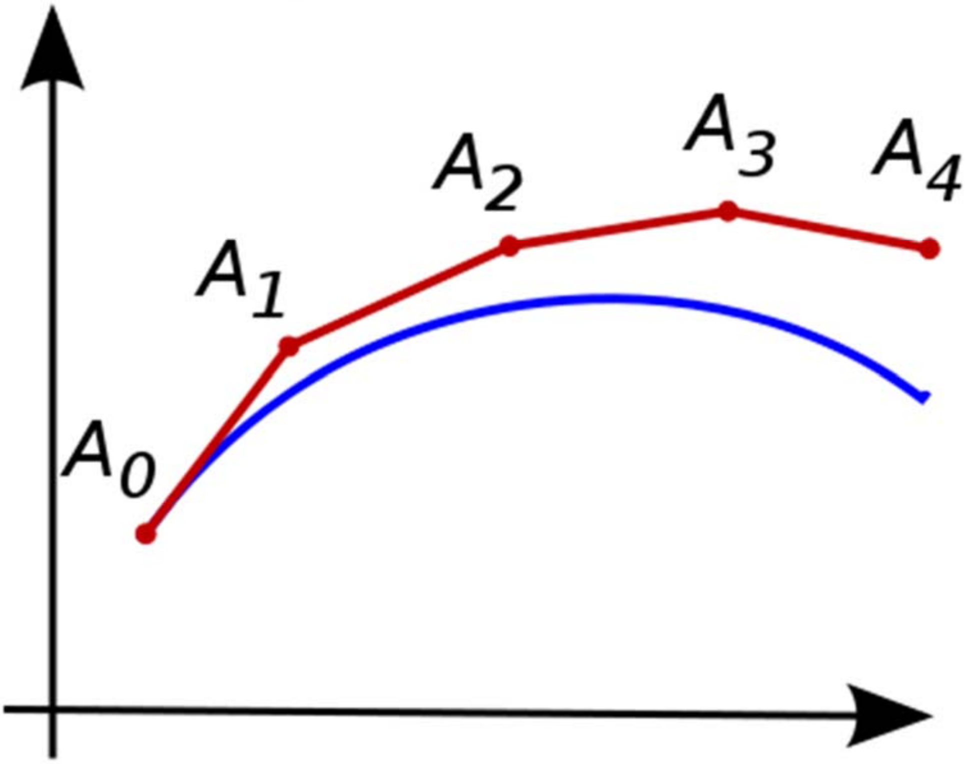
Start with y_0 and iterate:

$$y_{n+1} = y_n + \Delta t \cdot f(y_n, t_n) + O(\Delta^2 t)$$

This is the simplest finite difference method.

Since the error goes with $\Delta^2 t$ one needs a very small Δt and that is numerically very expensive.

Euler method



The order of a method

If the error at one time-step is $O(\Delta^n t)$ the method is „**locally of order *n***". To consider a fixed time interval T one needs $T/\Delta t$ time-steps so that the total error is:

$$\boxed{\frac{T}{\Delta t} O(\Delta^n t) = O(\Delta^{n-1} t)}$$

and therefore the method is „**globally of order *n*-1**".

The Euler method is globally of first order.

The Newton equation

$$\boxed{m\frac{d^2x}{dt^2} = F(x)}$$

2nd order ODE

Transform in a system of two coupled ODEs of first order.

$$\boxed{\begin{aligned}\frac{dx}{dt} &= v \\ \frac{dv}{dt} &= \frac{F(x)}{m}\end{aligned}}$$

Euler method for *N* coupled ODEs

N coupled ODEs of first order:

$$\boxed{\frac{dy_i}{dt} = f_i(y_1, \dots, y_N, t)\ , \quad i = 1, \dots, N}$$

iterate with a small Δt :

$$\boxed{y_i(t_{n+1}) = y_i(t_n) + \Delta t \cdot f_i(y_1(t_n), \dots, y_N(t_n), t_n) + O(\Delta^2 t)}$$

with $\boxed{t_n = t_0 + n \cdot \Delta t}$

Runge - Kutta method

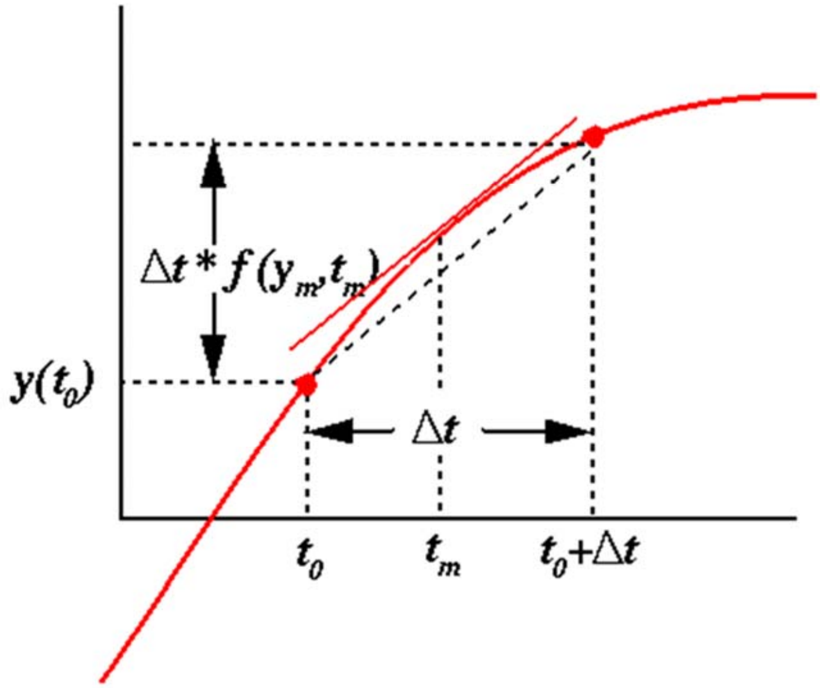
Carl David Tolmé Runge
(1856-1927)

Martin Wilhelm Kutta
(1867-1944)

References for R-K method

- G.E. Forsythe, M.A. Malcolm and C.B. Moler, „Computer Methods for Mathematical Computations“ (Prentice Hall, Englewood Cliffs, NJ, 1977), Chapter 6
- E. Hairer, S.P. Nørsett and G. Wanner, “Solving Ordinary Differential Equations I” (Springer, Berlin, 1993)
- W.H. Press, B.P.Flannery, S.A Teukolsky and W.T. Vetterling, “Numerical Recipes” (Cambridge University Press, Cambridge, 1988), Sect. 16.1 and 16.2
- J.C. Butcher, „The Numerical Analysis of Ordinary Differential Equations“ (Wiley, New York, 1987)
- J.D. Lambert, „Numerical Methods for Ordinary Differential Equations“ (John Wiley & Sons, New York, 1991)
- L.F. Shampine, „Numerical Solution of Ordinary Differential Equations“ (Chapman and Hall, London, 1994)

2nd order Runge - Kutta method



2nd order Runge - Kutta method

Extrapolate using Euler method to the value halfway, i.e. at $t + \Delta t / 2$:

$$\boxed{y_i(t + \frac{1}{2}\Delta t) = y_i(t) + \frac{1}{2}\Delta t \cdot f(y_i(t), t)}$$

Evaluate derivative in Euler method at this value:

$$\boxed{y_i(t + \Delta t) = y_i(t) + \Delta t \cdot f(y_i(t + \frac{1}{2}\Delta t), t + \frac{1}{2}\Delta t) + O(\Delta^3 t)}$$

Fourth order Runge - Kutta

$$k_1 = f(y_n, t_n)$$
$$k_2 = f(y_n + k_1/2, t_n + \Delta t/2)$$
$$k_3 = f(y_n + k_2/2, t_n + \Delta t/2)$$
$$k_4 = f(y_n + k_3, t_n + \Delta t)$$

RK4

applet

$$y_{n+1} = y_n + \Delta t\left(\frac{k_1}{6} + \frac{k_2}{3} + \frac{k_3}{3} + \frac{k_4}{6}\right) + O(\Delta^5 t)$$

RK4

- **k_1 is the slope at the beginning of the interval.**
- **k_2 is the slope at the midpoint of the interval, using slope k_1 to determine the value of y at the point $t_n+\Delta t/2$ using Euler method.**
- **k_3 is again the slope at the midpoint, but now using the slope k_2 to determine the y-value.**
- **k_4 is the slope at the end of the interval, with its y-value determined using slope k_3.**

Then use Euler method with

$$\text{slope} = \frac{k_1 + 2k_2 + 2k_3 + k_4}{6}$$

q-stage Runge - Kutta method

iteration:

$$\boxed{y_{n+1} = y_n + \Delta t \cdot \sum_{i=1}^{q} \omega_i k_i}$$

with

$$\boxed{k_i = f\left(y_n + \Delta t \sum_{j=1}^{i-1} \beta_{ij} k_j,\ \ t_n + \Delta t \alpha_i\right)}$$

and $\alpha_1 = 0$

explicit

implicit:

$$\boxed{k_i = f\left(y_n + \Delta t \sum_{j=1}^{q} \beta_{ij} k_j,\ \ t_n + \Delta t \alpha_i\right)}$$

q-stage Runge - Kutta method

$q = 1$ is the Euler method (unique)

Butcher array or Runge-Kutta tableau:

$$\begin{array}{c|ccccc}
\alpha_2 & \beta_{21} & & & & \\
\alpha_3 & \beta_{31} & \beta_{32} & & & \\
\vdots & \vdots & & \ddots & & \\
\alpha_q & \beta_{q1} & \beta_{q2} & \cdots & \beta_{q,q-1} & \\
\hline
 & \omega_1 & \omega_2 & \cdots & \omega_{q-1} & \omega_q
\end{array}$$

resumes all parameters of the general Runge-Kutta

Example RK4

Butcher array:

0				
½	½			
½	0	½		
1	0	0	1	
	$\frac{1}{6}$	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{6}$

its stage is: $q = 4$

RK4 is of order $p = 4$

Order of Runge - Kutta method

The R-K method is of order p if:

$$\boxed{y(t+\Delta t) - y(t) - \Delta t \cdot \sum_{i=1}^{q} \omega_i k_i = O(\Delta t^{p+1})}$$

One must choose the α_i, β_{ij} and ω_i for $i,j \in [1, q]$ such that the left hand side = 0 in $O(\Delta t^m)$ for all $m \le p$.

Taylor expansion:

$$\boxed{y(t+\Delta t) - y(t) = \sum_{m=1}^{p} \frac{1}{m!} \Delta t^m \cdot \left[\frac{d^{m-1} f}{dt^{m-1}}\right]_{y(t),t} + O(\Delta t^{p+1})}$$

Order of Runge - Kutta method

$$\Rightarrow \sum_{i=1}^{q} \omega_i k_i = \sum_{m=1}^{p} \frac{1}{m!} \Delta t^{m-1} \cdot \left[\frac{d^{m-1} f}{dt^{m-1}} \right]_{y(t),t}$$

up to $O(\Delta t^{\,p+1})$

Example $q = p = 1$: $\omega_1 \cdot f(y_n, t_n) = f(y_n, t_n) \Rightarrow \omega_1 = 1$

$\Rightarrow$ gives Euler method.

Example $q = p = 2$: $\omega_1 \cdot k_1 + \omega_2 \cdot k_2 = f_n + \frac{1}{2} \Delta t \left[\frac{df}{dt} \right]_n$

where index „n“ means „at (y_n, t_n)“.

Example $q = p = 2$

$$\omega_1 \cdot k_1 + \omega_2 \cdot k_2 = f_n + \frac{1}{2} \Delta t \left[\frac{df}{dt} \right]_n = f_n + \frac{1}{2} \Delta t \left(\left[\frac{\partial f}{\partial t} \right]_n + \left[\frac{\partial f}{\partial y} \right]_n \cdot f_n \right)$$

insert

$$k_1 = f(y_n, t_n) \equiv f_n$$
$$k_2 = f(y_n + \Delta t \cdot \beta_{21} \cdot k_1,\; t_n + \Delta t \cdot \alpha_2)$$
$$= f_n + \Delta t \cdot \beta_{21} \cdot \left[\frac{\partial f}{\partial y} \right]_n \cdot f_n + \Delta t \cdot \alpha_2 \cdot \left[\frac{\partial f}{\partial t} \right]_n + O(\Delta t^2)$$

$$\Rightarrow \quad \omega_1 + \omega_2 = 1 \;,\quad \omega_2 \cdot \alpha_2 = \frac{1}{2} \;,\quad \omega_2 \cdot \beta_{21} = \frac{1}{2}$$

3 equations for 4 parameters $\Rightarrow$ one-parameter family

Example $q = p = 2$

$$y_{n+1} = y_n + \Delta t \cdot \left[(1-\omega_2) \cdot k_1 + \omega_2 k_2 \right]$$

$$k_1 = f(y_n, t_n)$$

$$k_2 = f\left(y_n + \frac{\Delta t}{2\omega_2}, t_n + \frac{\Delta t}{2\omega_2}\right)$$

Order of Runge - Kutta method

To obtain a Runge-Kutta method of given order p one needs a minimum stage of $q_{\min}$.

p	1	2	3	4	5	6	7	8	9	10
$q_{\min}$	1	2	3	4	6	7	9	11	12 – 17	13 - 17

John Butcher

Example: Lorenz equation

Is a simplified system of equations describing the 2-dimensional flow of fluid of uniform depth in the presence of an imposed temperature difference taking into account gravity, buoyancy, thermal diffusivity, and kinematic viscosity (friction).

σ Prandtl number
ρ Rayleigh number
$\sigma = 10$, $\beta = 8/3$
ρ is varied.
Chaos for $\rho = 28$.

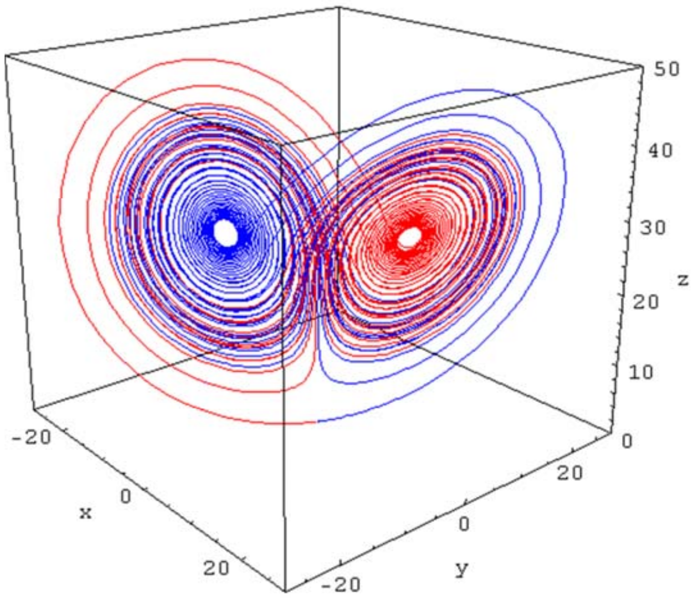
$$y_1' = \sigma (y_2 - y_1)$$
$$y_2' = y_1 (\rho - y_3) - y_2$$
$$y_3' = y_1 y_2 - \beta y_3$$

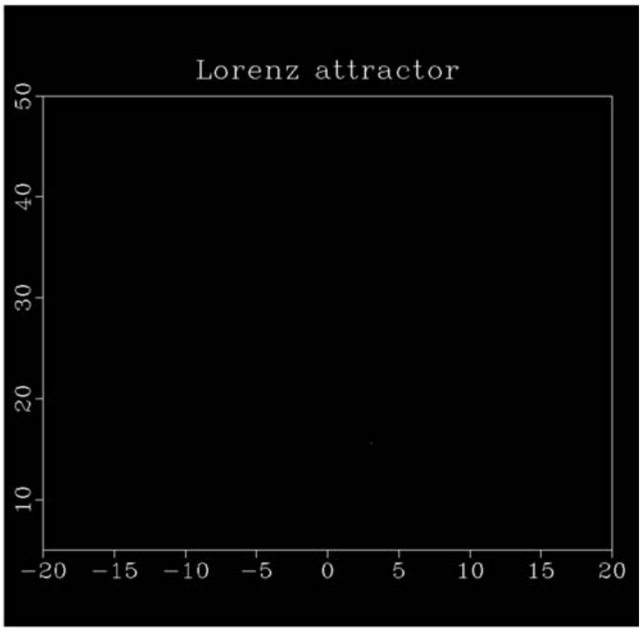
Edward Norton Lorenz (1963)

applet

C.Sparrow: „The Lorenz Equations: Bifurcations, Chaos and Strange Attractors“ (Springer Verlag, N.Y., 1982)

Lorenz attractor





Example: Lorenz equation

Chaotic solutions of the Lorenz equation exist and are not numerical artefacts (14th math problem of Smale).

Warwick Tucker (2002)

Ordinary differential equations

First order ODE, initial value problem:

$$\boxed{\frac{dy}{dt} = f(y,t)} \quad \text{with } y(t_0) = y_0$$

examples:

radioactive decay $\boxed{\frac{dN}{dt} = -\lambda N}$

coffee cooling $\boxed{\frac{dT}{dt} = -\gamma(T - T_{room})}$

Explicit forward integration

Euler method

Start with y_0 and iterate:

$$\boxed{y_{n+1} = y_n + \Delta t \cdot f(y_n, t_n) + O(\Delta^2 t)}$$

This is the simplest finite difference method.

Since the error goes with $\Delta^2 t$ one needs a very small Δt and that is numerically very expensive.

Error reduction

Let us consider a method of order p, (error = $\Phi \Delta t^{p+1}$).

Be y_1 the predicted value for $2\Delta t$

and y_2 the predicted value making two steps Δt.

Define difference as $\delta = y_2 - y_1$

$$y(t + 2\Delta t) = \begin{cases} y_1 + (2\Delta t)^{p+1}\Phi + O(\Delta t^{p+2}) \\ y_2 + 2\boxed{\dfrac{\delta}{\left(2^{p+1} - 2\right)}} + O(\Delta t^{p+2}) \end{cases}$$

$$\Rightarrow \delta = (2^{p+1} - 2)\boxed{\Delta t^{p+1}\Phi} + O(\Delta t^{p+2})$$

Error reduction

improve systematically:

$$\boldsymbol{y}(\boldsymbol{t}+\Delta\boldsymbol{t}) = \boldsymbol{y}_2 + \frac{2\delta}{2^{\boldsymbol{p}+1}-2} + \boldsymbol{O}(\Delta\boldsymbol{t}^{\boldsymbol{p}+2})$$

example RK4:

$$\boldsymbol{y}(\boldsymbol{t}+\Delta\boldsymbol{t}) = \boldsymbol{y}_2 + \frac{\delta}{15} + \boldsymbol{O}(\Delta\boldsymbol{t}^{\boldsymbol{p}+2})$$

Error reduction

General for two different time steps Δt_1 and Δt_2

$$y = y_{\Delta t_i^{p+1}} + \Phi \Delta t_i^{p+1} + O\left(\Delta t_i^{p+2}\right) \quad , \quad i = 1,2$$

$$\left(\Delta t_2^{p+1} - \Delta t_1^{p+1}\right) y = \Delta t_2^{p+1} y_{\Delta t_1^{p+1}} - \Delta t_1^{p+1} y_{\Delta t_2^{p+1}} + O\left(\Delta t_i^{p+2}\right)$$

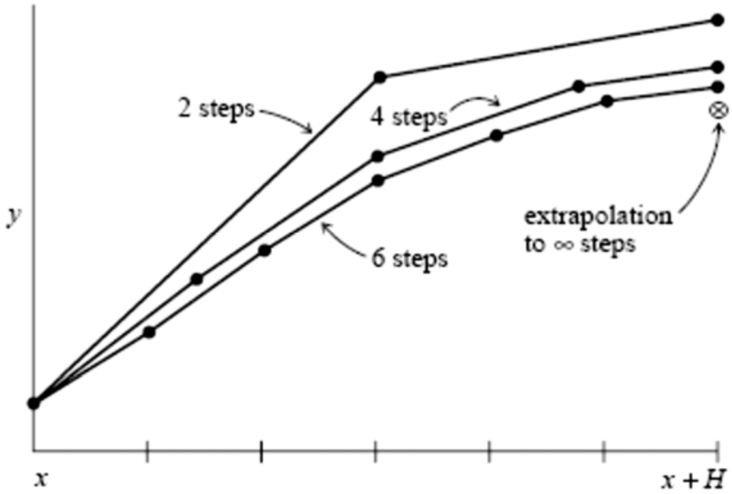
$$y = \frac{\Delta t_2^{p+1} y_{\Delta t_1^{p+1}} - \Delta t_1^{p+1} y_{\Delta t_2^{p+1}}}{\Delta t_2^{p+1} - \Delta t_1^{p+1}} + O\left(\Delta t_i^{p+2}\right)$$

Richardson extrapolation

Lewis Fry Richarson

Calculate for various Δt_i and extrapolate

$$y = \lim_{\Delta t_i \to 0} y_{\Delta t_i}$$



Bulirsch - Stoer Method

Extrapolate with rational function:

$$y_{\Delta t_n} = \frac{p_0 + p_1 \Delta t_n + \ldots + p_k \left(\Delta t_n\right)^k}{q_0 + q_1 \Delta t_n + \ldots + q_m \left(\Delta t_n\right)^m} \xrightarrow[\Delta t_n \to 0]{} y$$

$$\Delta t_n = \frac{\Delta t}{n} \quad , \qquad n = 2, 4, 6, 8, 12, 16, 24, 32, 48, 64, 96, \ldots$$

Choose k and m appropiately.

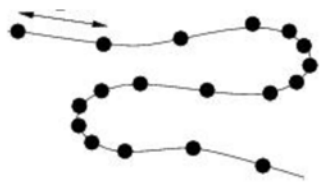
R. Bulirsch and J. Stoer, „Introduction to Numerical Analysis“ (Springer, NY, 1992)

Adaptive time-step Δt

Define the error $\delta_{expected}$ you want to accept. Then measure the real error $\delta_{measured}$ and define a new time-step through:

$$\Delta t_{new} = \Delta t_{old} \left(\frac{\delta_{expected}}{\delta_{measured}} \right)^{\frac{1}{p+1}}$$

because $\delta = \phi \, \Delta t^{\,p+1}$.



Predictor-corrector method

idea:

$$y(t+\Delta t) \approx y(t) + \Delta t \cdot \frac{f(y(t)) + f(y(t+\Delta t))}{2}$$

implicit equation

make prediction using Taylor:

$$y^P(t+\Delta t) = y(t) + \Delta t \cdot \frac{dy}{dt}(t) + O(\Delta t^2)$$

correct by inserting:

$$y^C(t+\Delta t) = y(t) + \frac{\Delta t}{2}[f(y(t)) + f(y^P(t+\Delta t))] + O(\Delta t^3)$$

Can be iterated by again inserting corrected value.

3th order predictor-corrector

Predict through 3rd order Taylor expansion:

$$y^P(t+\Delta t) = y(t) + \Delta t \cdot \frac{dy}{dt}(t) + \frac{\Delta t^2}{2} \cdot \frac{d^2y}{dt^2}(t) + \frac{\Delta t^3}{6} \cdot \frac{d^3y}{dt^3}(t) + O(\Delta t^4)$$

$$\left(\frac{dy}{dt}\right)^P (t+\Delta t) = \frac{dy}{dt}(t) + \Delta t \cdot \frac{d^2y}{dt^2}(t) + \frac{\Delta t^2}{2} \cdot \frac{d^3y}{dt^3}(t) + O(\Delta t^3)$$

$$\left(\frac{d^2y}{dt^2}\right)^P (t+\Delta t) = \frac{d^2y}{dt^2}(t) + \Delta t \cdot \frac{d^3y}{dt^3}(t) + O(\Delta t^2)$$

$$\left(\frac{d^3y}{dt^3}\right)^P (t+\Delta t) = \frac{d^3y}{dt^3}(t) + O(\Delta t)$$

3th order predictor- corrector

use equation: $$\left(\frac{dy}{dt}\right)^C (t+\Delta t) = f(y^P(t+\Delta t))$$

define error: $$\delta = \left(\frac{dy}{dt}\right)^C (t+\Delta t) - \left(\frac{dy}{dt}\right)^P (t+\Delta t)$$

correct:

$$y^C(t+\Delta t) = y^P + c_0 \cdot \delta$$

$$\left(\frac{d^2y}{dt^2}\right)^C (t+\Delta t) = \left(\frac{d^2y}{dt^2}\right)^P + c_2 \cdot \delta$$

$$\left(\frac{d^3y}{dt^3}\right)^C (t+\Delta t) = \left(\frac{d^3y}{dt^3}\right)^P + c_3 \cdot \delta$$

Procedure can be repeated.

Charles William Gear

Gear coefficients:

$c_0 = 3/8$

$c_2 = 3/4$

$c_3 = 1/6$

5th order predictor- corrector

Be $\mathbf{r}_0 \equiv y$. Then one can define the time derivatives:

$$\mathbf{r}_1 = \partial t(d\mathbf{r}_0/dt),\ \mathbf{r}_2 = 1/2\partial t^2(d^2\mathbf{r}_0/dt^2),\ \mathbf{r}_3 = 1/6\partial t^3(d^3\mathbf{r}_0/dt^3),\ \text{etc.}$$

Predictor:

$$\begin{pmatrix} \mathbf{r}_0^p(t+\partial t) \\ \mathbf{r}_1^p(t+\partial t) \\ \mathbf{r}_2^p(t+\partial t) \\ \mathbf{r}_3^p(t+\partial t) \\ \mathbf{r}_4^p(t+\partial t) \\ \mathbf{r}_5^p(t+\partial t) \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & 2 & 3 & 4 & 5 \\ 0 & 0 & 1 & 3 & 6 & 10 \\ 0 & 0 & 0 & 1 & 4 & 10 \\ 0 & 0 & 0 & 0 & 1 & 5 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \mathbf{r}_0(t) \\ \mathbf{r}_1(t) \\ \mathbf{r}_2(t) \\ \mathbf{r}_3(t) \\ \mathbf{r}_4(t) \\ \mathbf{r}_5(t) \end{pmatrix}$$

5th order predictor- corrector

1st order eq.: $$\frac{d\mathbf{r}}{dt} = f(\mathbf{r}) \Rightarrow \mathbf{r}_1^C = f(\mathbf{r}_0^P) \Rightarrow \Delta\mathbf{r} = \mathbf{r}_1^C - \mathbf{r}_1^P$$

2nd order eq.: $$\frac{d^2\mathbf{r}}{dt^2} = f(\mathbf{r}) \Rightarrow \mathbf{r}_2^C = 2f(\mathbf{r}_0^P) \Rightarrow \Delta\mathbf{r} = \mathbf{r}_2^C - \mathbf{r}_2^P$$

Corrector:

$$\begin{pmatrix} \mathbf{r}_0^c(t+\partial t) \\ \mathbf{r}_1^c(t+\partial t) \\ \mathbf{r}_2^c(t+\partial t) \\ \mathbf{r}_3^c(t+\partial t) \\ \mathbf{r}_4^c(t+\partial t) \\ \mathbf{r}_5^c(t+\partial t) \end{pmatrix} = \begin{pmatrix} \mathbf{r}_0^p(t+\partial t) \\ \mathbf{r}_1^p(t+\partial t) \\ \mathbf{r}_2^p(t+\partial t) \\ \mathbf{r}_3^p(t+\partial t) \\ \mathbf{r}_4^p(t+\partial t) \\ \mathbf{r}_5^p(t+\partial t) \end{pmatrix} + \begin{pmatrix} c_0 \\ c_1 \\ c_2 \\ c_3 \\ c_4 \\ c_5 \end{pmatrix} \cdot \Delta\mathbf{r}$$

Gear coefficients (1971)

1st order equation:

Value	c_0	c_1	c_2	c_3	c_4	c_5
3	5/12	1	1/2			
4	3/8	1	3/4	1/6		
5	251/720	1	11/12	1/3	1/24	
6	95/288	1	25/24	35/72	5/48	1/120

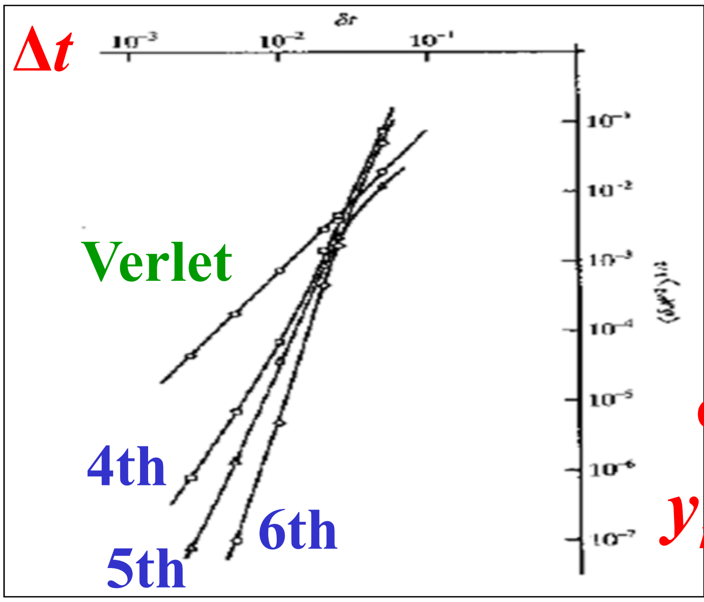
2nd order equation:

Value	c_0	c_1	c_2	c_3	c_4	c_5
3	0	1	1			
4	1/6	5/6	1	1/3		
5	19/120	3/4	1	1/2	1/12	
6	3/20	251/360	1	11/18	1/6	1/60

Function	c_0	c_1	c_2	c_3	c_4	c_5
$\dot{\mathbf{r}} = f(\mathbf{r})$	95/288	1	25/24	35/72	5/48	1/120
$\ddot{\mathbf{r}} = f(\mathbf{r})$	3/20	251/360	1	11/18	1/6	1/60
$\ddot{\mathbf{r}} = f(\mathbf{r}, \dot{\mathbf{r}})$	3/16	251/360	1	11/18	1/6	1/60

Comparison of methods

for fixed number of iterations *n*



error

$y_{n+1} - y_n$

Predictor - Corrector

Sets of coupled ODEs

Explicit Runge Kutta and Predictor Corrector methods can be straightforwardly generalized to a set of coupled 1st order ODEs:

$$\frac{dy_i}{dt} = f_i(y_1, ..., y_N, t) \ , \quad i = 1, ..., N$$

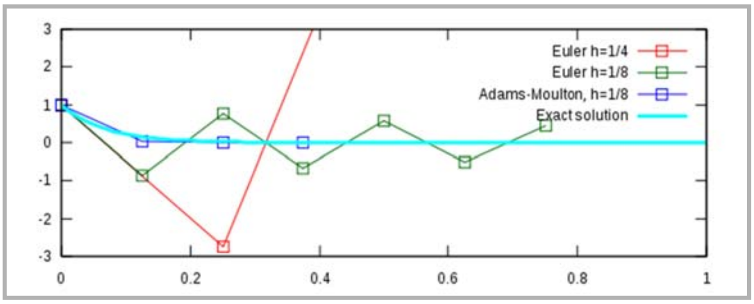
by inserting simultaneously all the values of the previous iteration.

Stiff differential equation

example: $y'(t) = -15 y(t) \ , \ t \geq 0 \ , \ y(0) = 1$

Euler: $y(t+\Delta t) = y(t) - \Delta t \ 15 \ y(t) + O(\Delta t^2)$

Becomes unstable if Δt not small enough:



Use implicit method: **(e.g. Adams – Moulton)**

$$y(t+\Delta t) = y(t) + \frac{1}{2}\Delta t \ \left(f(y(t), t) + f(y(t+\Delta t), t+\Delta t) \right) + O(\Delta t^2)$$

Stiff sets of equations

ETH

$$\boxed{\vec{y}'(t) = \overleftrightarrow{K} \cdot \vec{y}(t) + \vec{f}(t)}$$

This system is called „stiff“ if matrix $\overleftrightarrow{K}$ has at least one very large eigenvalue.

$$\boxed{\vec{y}'(t) = \vec{f}(\vec{y}(t), t)}$$

This system is called „stiff“ if Jacobi matrix has at least one very large eigenvalue.

example:

$$\boxed{\begin{array}{l} y_1' = 1000\, y_1 + y_2 \\ y_2' = 999\, y_1 \\ y_1(0) = 1 \;\;,\;\; y_2(0) = 1 \end{array}}$$

Solve with with implicit method.