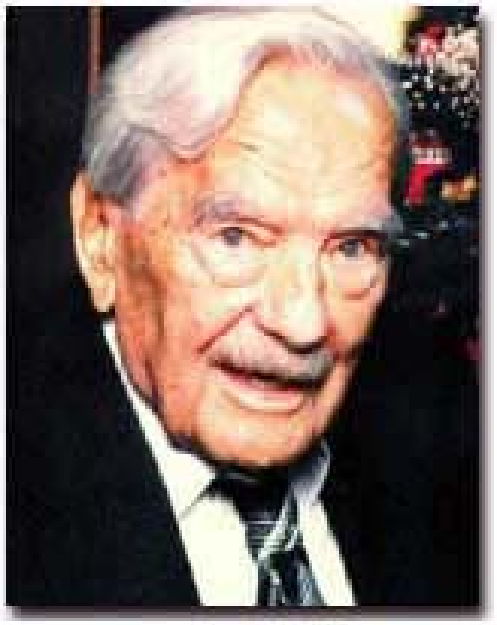
Monte Carlo Methods



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:

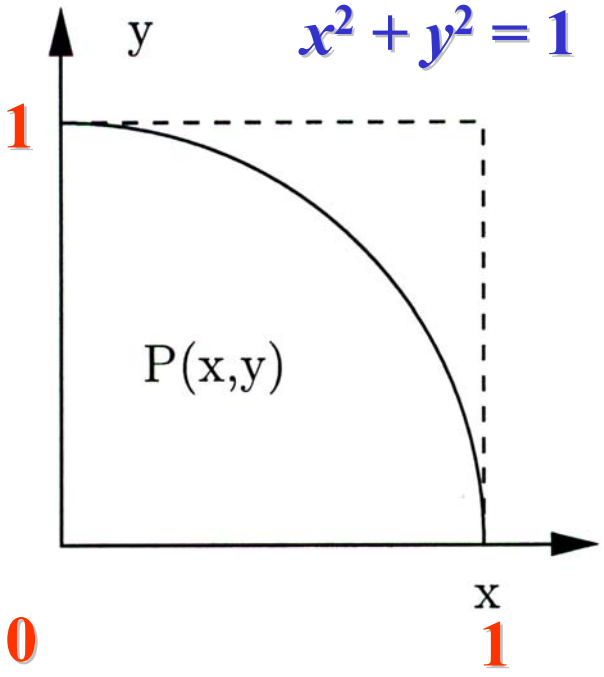
Systematic improvement by increasing the number of samples N.

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

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

$c = 0$

if $y_i^2 < 1 - x_i^2 \Rightarrow c = c + 1$

c is number of points that fall inside circle.

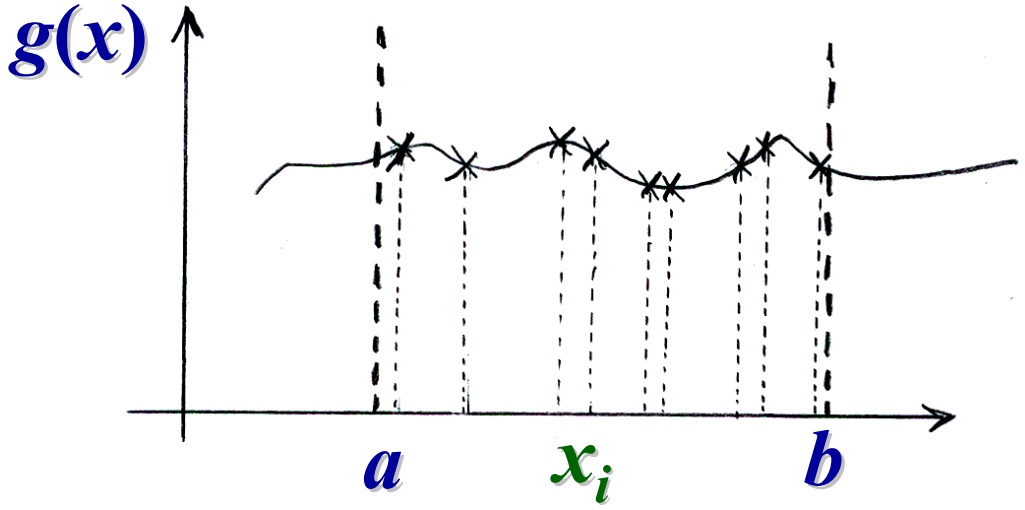
area $\propto c/N$

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

applet

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

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“

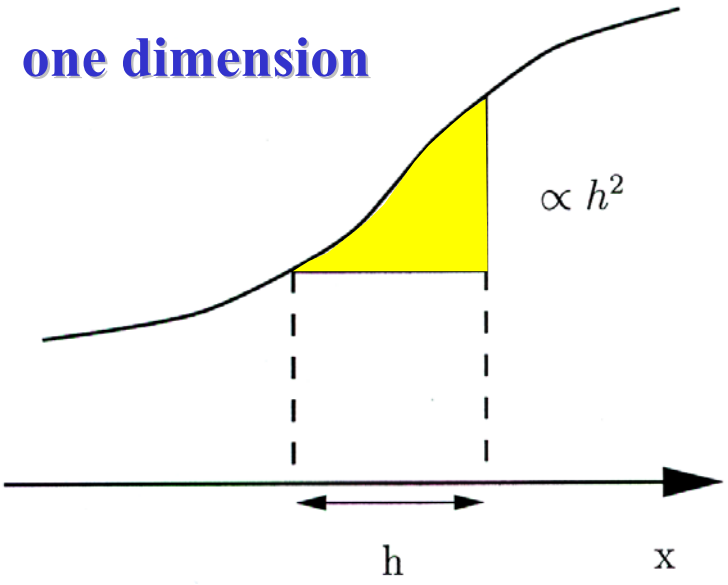
Good if $g(x)$ smooth.

Error of integration

conventional method:

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

one dimension



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

where T is the computer time.

error:

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

Error in d dimensions

in d dimensions:

$$h \propto \frac{1}{L} \quad , \quad T \propto N = L^d \quad \Rightarrow \quad h \propto T^{-\frac{1}{d}}$$

error with conventional method:

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

error with Monte Carlo:

$$\Delta \propto \frac{1}{\sqrt{N}} \propto T^{-\frac{1}{2}}$$

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

High dimensional integral

ETH

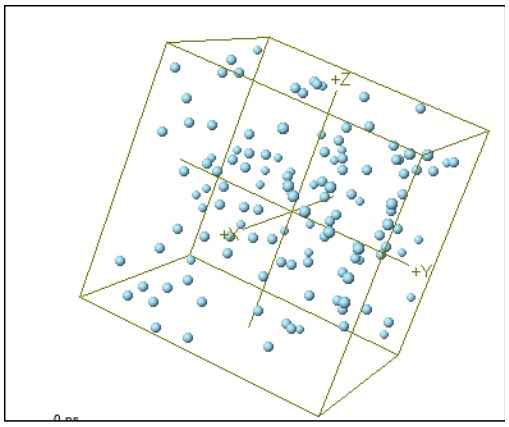
Consider *n* hard spheres of radius *R* in a 3*d* box.

Phase space is 3*n* 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:

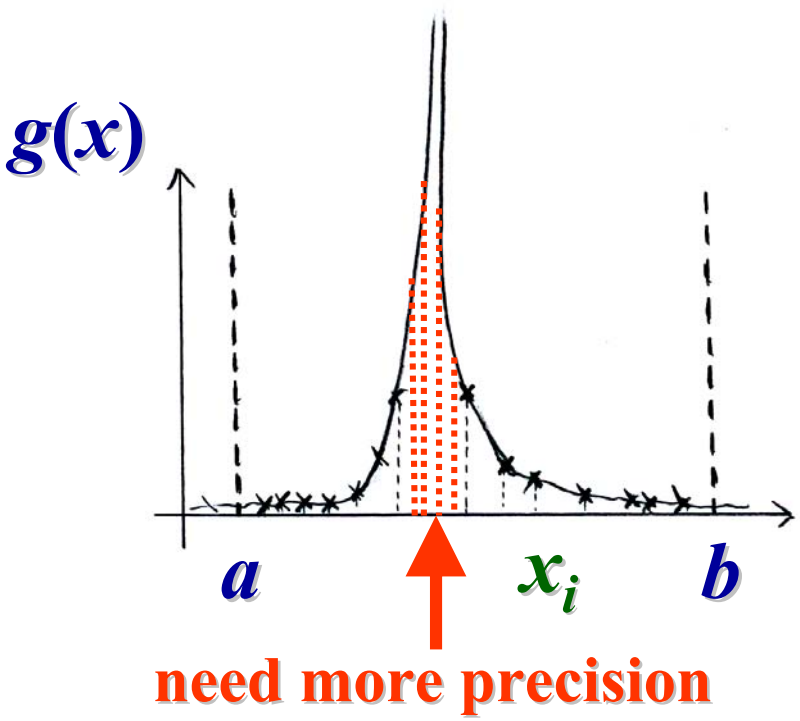
$$< r_{ij} >= \frac{1}{Z} \int \frac{2}{n(n-1)} \sum_{i<j} r_{ij} dx_1, .., dx_n dy_1, .., dy_n dz_1, .., dz_n$$

MC strategy

ETH

- **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

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

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

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

„importance sampling“

Canonical Monte Carlo

ETH

$E(X)$ = 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:

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

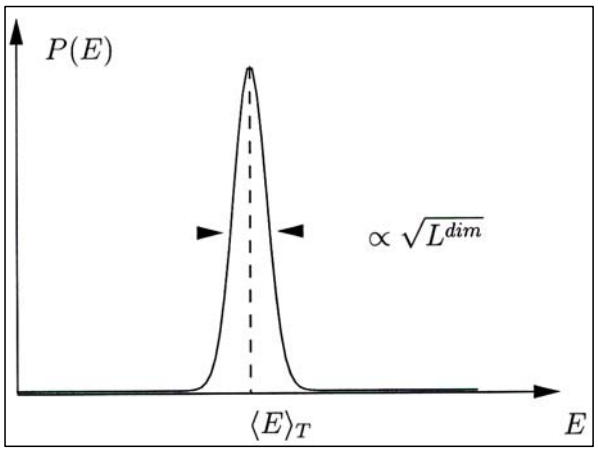
$$\sum_X p_{eq}(X) = 1$$

Problem of sampling

ETH

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

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

ETH

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-1}

Properties of Markov chain

ETH

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:

$$\sum_Y T(X \rightarrow Y) = 1$$

3. Reversibility:

$$T(X \rightarrow Y) = T(Y \rightarrow X)$$

Transition probability

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

Total probability of Markov chain is:

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

Master equation:

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

Properties of $W(X \to Y)$

- **Ergodicity:**

$$\forall X, Y : W(X \to Y) > 0$$

- **Normality:**

$$\sum_Y W(X \to Y) = 1$$

- **Homogeneity:**

$$\sum_Y p_{st}(Y)\, W(Y \to X) = p_{st}(X)$$

Detailed balance

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

In stationary state one should have equilibrium distribution (Boltzmann)

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

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

sufficient condition is detailed balance:

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

Metropolis ($M(RT)^2$)

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

Boltzmann:

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

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

If energy decreases always accept

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

Glauber dynamics

ETH

Roy C. Glauber (1963)

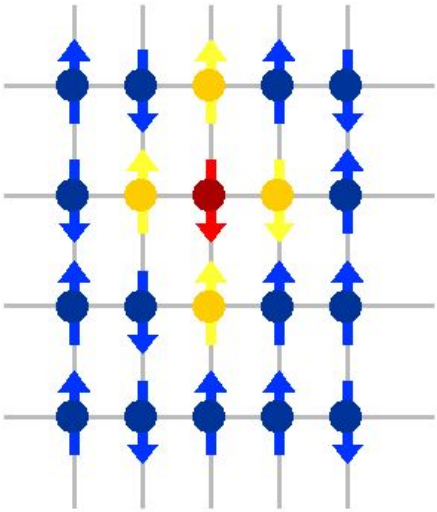
(Nobel prize 2005)

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

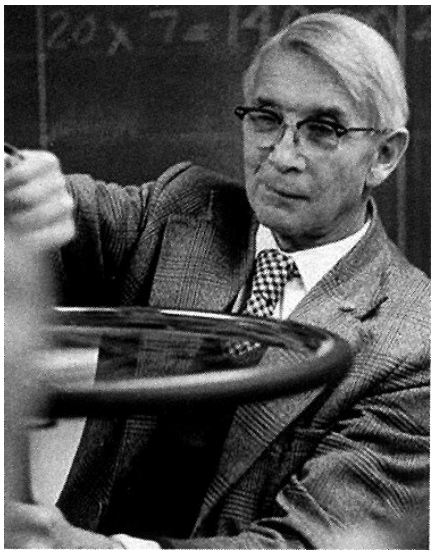
also fulfills detailed balance

The Ising Model

ETH



Spins on a lattice



Ernst Ising (1900-1998)

- Magnetic Systems
- Opinion models
- Binary mixtures

The Ising Model

ETH

Binary variables:

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

on a graph of *N* sites

interacting via the Hamiltonian:

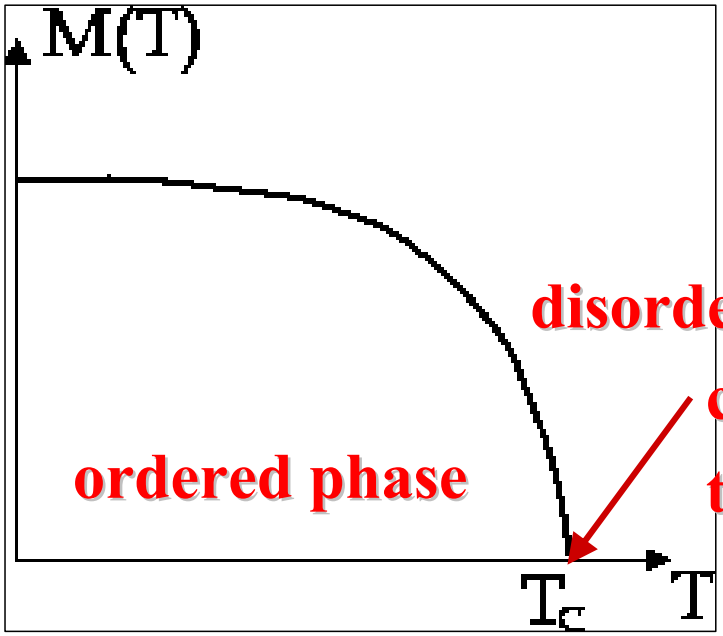
$$\mathcal{H} = E = -J \sum_{i,j:nn} \sigma_i \sigma_j - H \sum_{i=1}^{N} \sigma_i$$

Order parameter

ETH

spontaneous magnetization:

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



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

disordered phase

critical temperature

ordered phase

$\beta = 1/8 \quad (2d)$

$\beta \approx 0.326 \; (3d)$

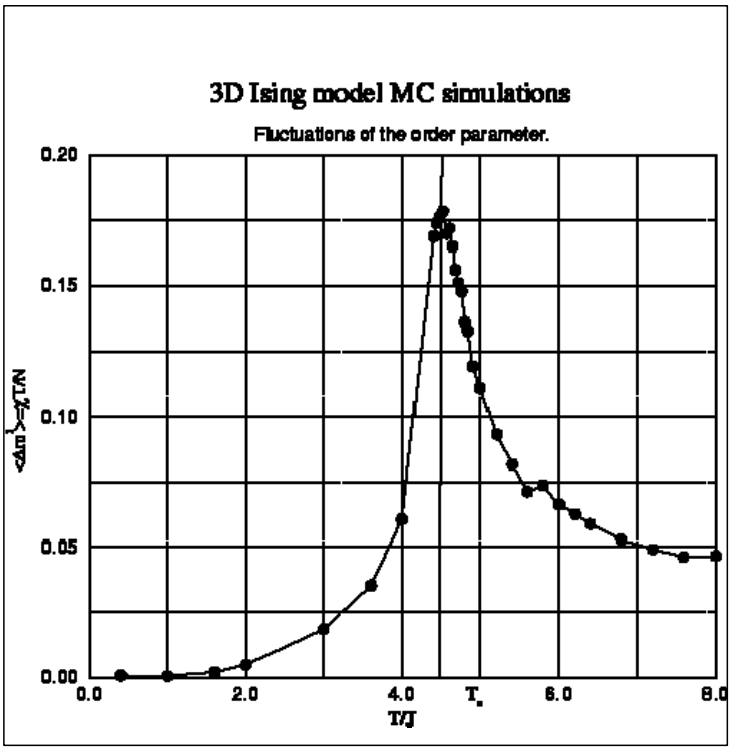
Susceptibility

ETH

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

$\gamma = 7/4$ (2d)

$\gamma \approx 1.24$ (3d)



numerical data from a finite system

MC of the Ising Model

ETH

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: $\sigma_i \rightarrow -\sigma_i$.
- If $\Delta E > 0$ flip with probability $\exp(-\Delta E/kT)$.

where h_i is the local field at site i

$$h_i = \sum_{nn\ of\ i} \sigma_j$$

applet

Binary mixtures
(lattice gas)

ETH

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.

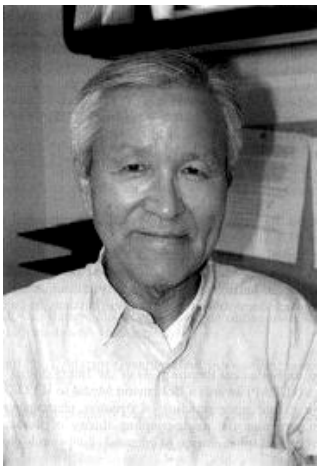
Set $E_{AA} = E_{BB} = 0$ and $E_{AB} = 1$.

Number of each species is constant.

Kawasaki dynamics

ETH

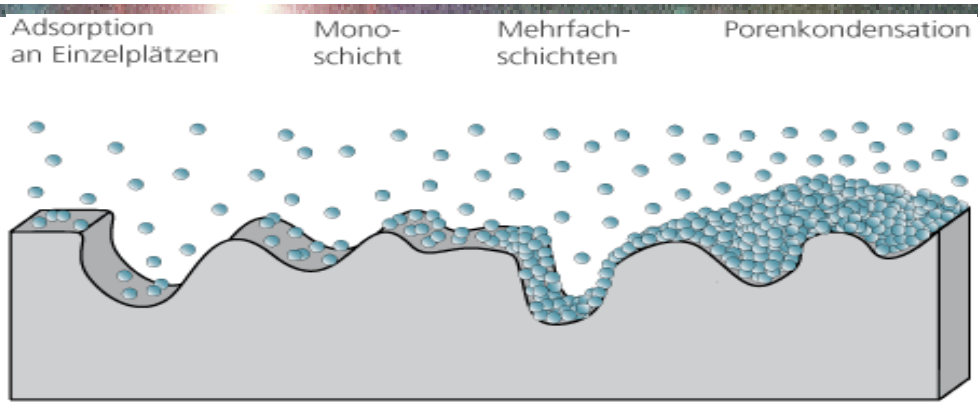
- Choose any A-B bond.
- Calculate ΔE for A-B → B-A.
- **Metropolis:** If $\Delta E \leq 0$ flip, else flip with $p = \exp(-\beta \Delta E)$.
- **Glauber:** Flip with probability $p = \exp(-\beta \Delta E)/(1+\exp(-\beta \Delta E))$.



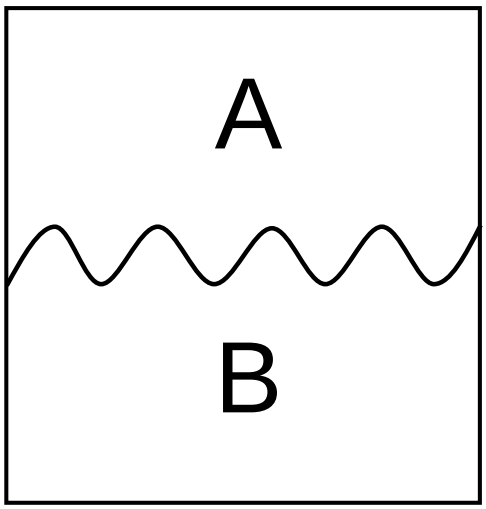
Kyozi Kawasaki

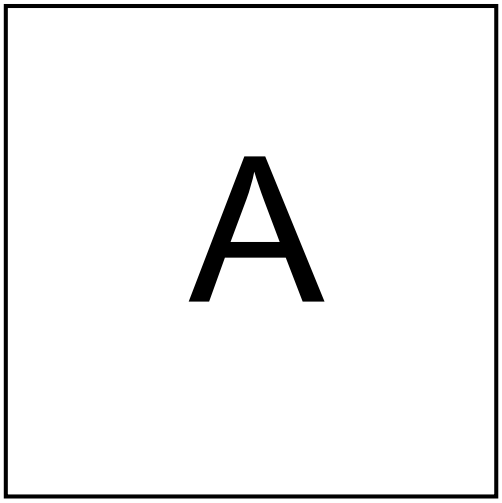
$$\beta = 1/kT$$

Interfaces



Interfaces





surface tension

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

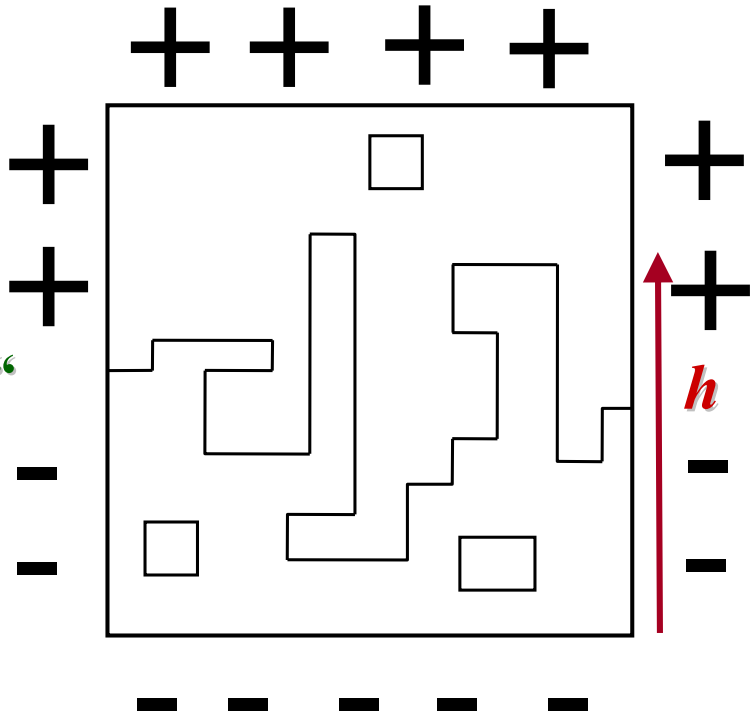
Ising interface

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

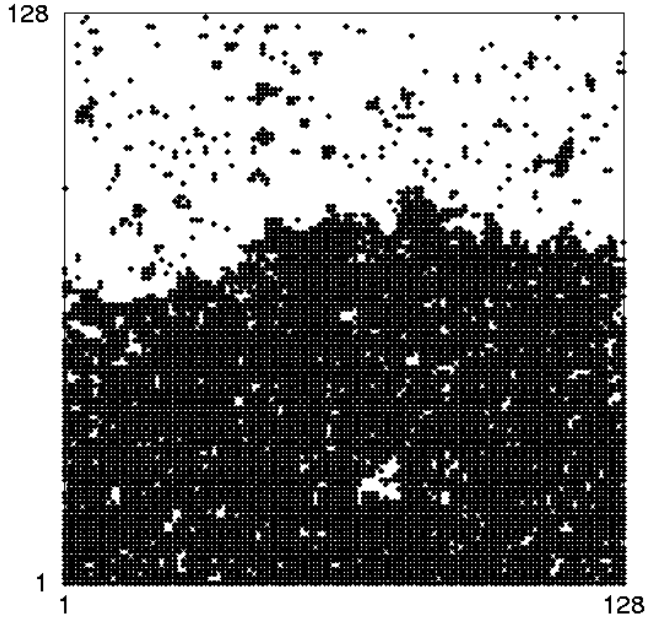
Fixed boundary conditions:

upper half „+“, lower half „–“

Simulate with Kawasaki dynamics at temperature *T*.

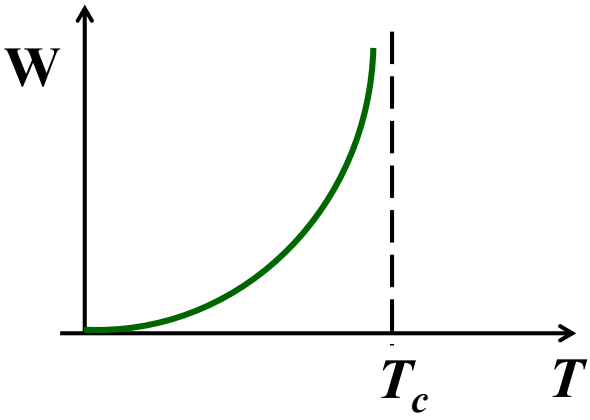


Ising interface



interface width *W*:

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



roughening transition

Self-affine scaling

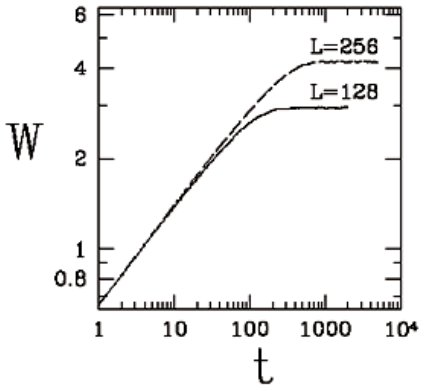


Figure 1. Interface width W versus time t for the RSOS model (Ref. [11]) in $1+1$ dimensions, in two different lattice lengths L.

Family-Vicsek scaling (1985):

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

ξ is the roughening exponent, z the dynamic exponent.

Self-affine scaling

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

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

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

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

$$\Rightarrow \quad \beta = \frac{\xi}{z}$$

β is the growth exponent.

Numerically these laws are verified by data collapse.

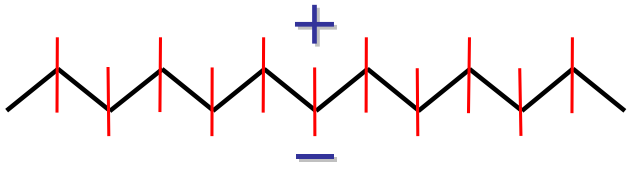
Ising interface

ETH

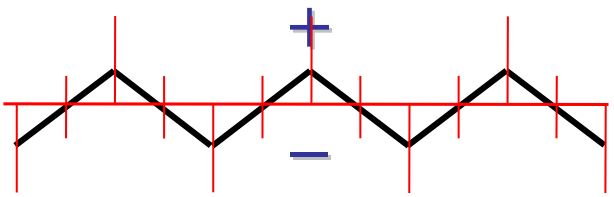
Add next-nearest neighbor interaction:

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

punishes curvature ↔ introduces stiffness



$11 \times K$



$17 \times K$

Shape of drop

ETH

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

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

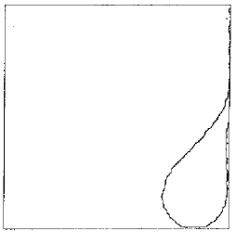
with $h_j = h_1 + \dfrac{(j-1)(h_L - h_1)}{L-1}$ and $g = \dfrac{h_L - h_1}{L}$

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

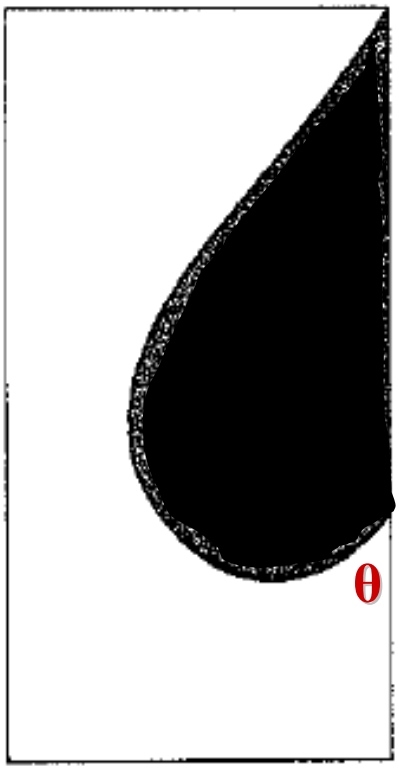
Shape of drop

ETH

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



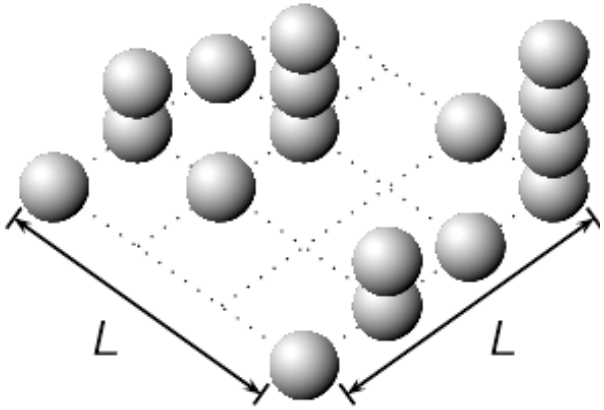
Contact angle θ is function of temperature and vanishes when approaching T_c.



Solid on solid model (SOS)

ETH

adatoms and
surface growth



interface without islands and without overhangs

$$\mathcal{H} = E = -\varepsilon \sum_{i,j:nn}^{N} \left| h_i - h_j \right|$$

Irreversible growth

ETH

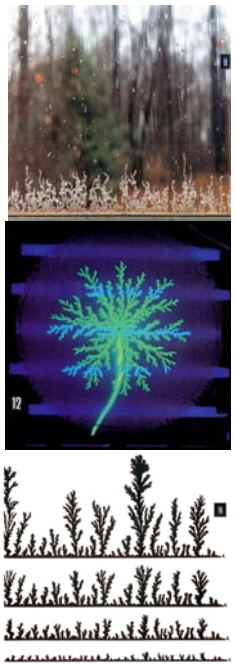
- T. Vicsek, „Fractal Growth Phenomena“ (World Scientific, Singapore, 1989
- A.-L. Barabasi and H.E. Stanley, „Fractal Concepts in Surface Growth“ (Cambridge Univ. Press, 1995)
- H.J. Herrmann, „Geometric Cluster Growth Models and Kinetic Gelation“, Phys. Rep. 136, 153 (1986)

Irreversible growth

ETH

No thermal equilibrium

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



Random deposition

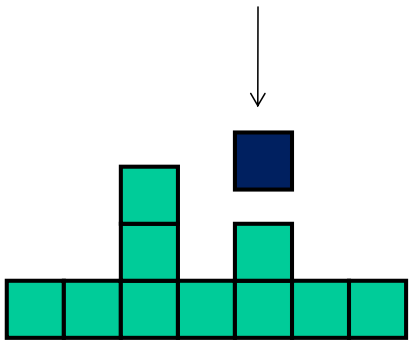
Random deposition

simplest possible growth model

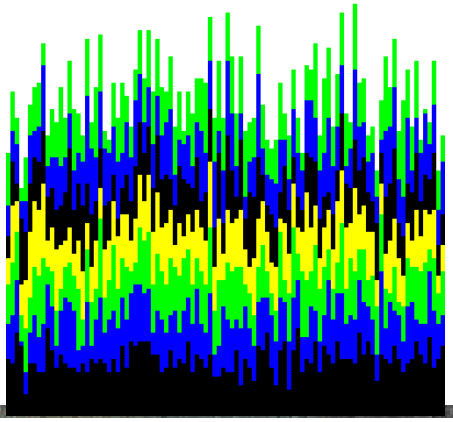
$$\langle h \rangle \sim t$$

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

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



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



Random deposition with surface diffusion

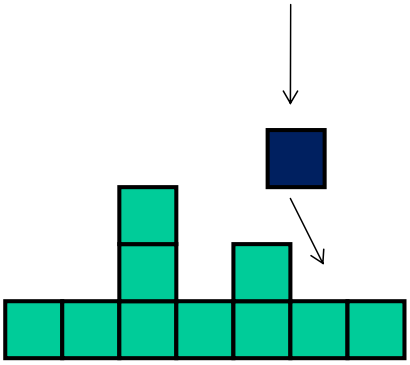
Particle can move a short distance to find a more stable configuration.

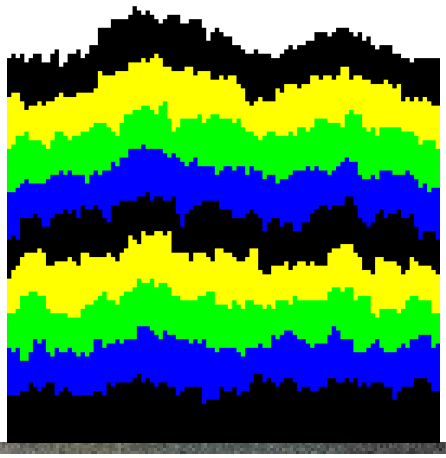
$$\langle h \rangle \sim t$$

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

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.

$$\beta = 1/4$$
$$\xi = 1/2$$



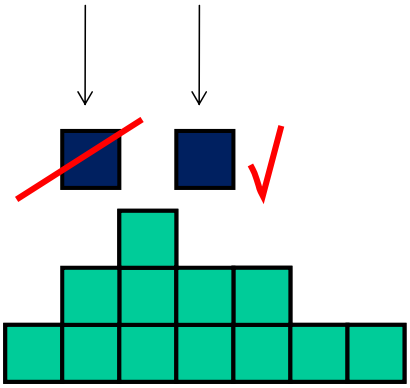


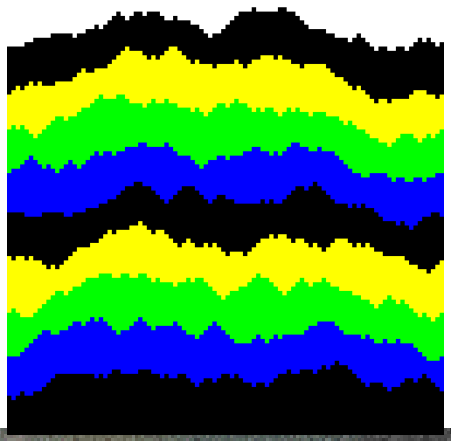
Restricted Solid On Solid Model (RSOS)

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

Pick a random column i.
Add a particle only if
$h(i) \leq h(i-1)$ and $h(i) \leq h(i+1)$.
Otherwise pick a new column.

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





Eden model

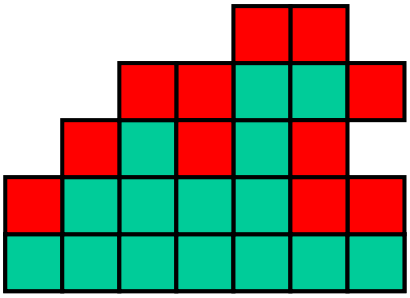
ETH

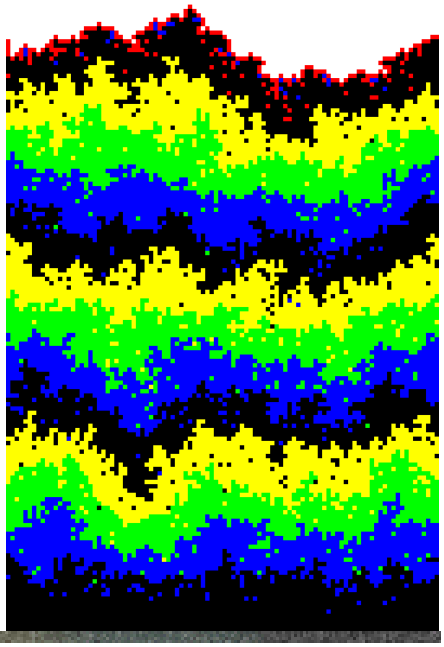
simple model for tumor growth or epidemic spread

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….

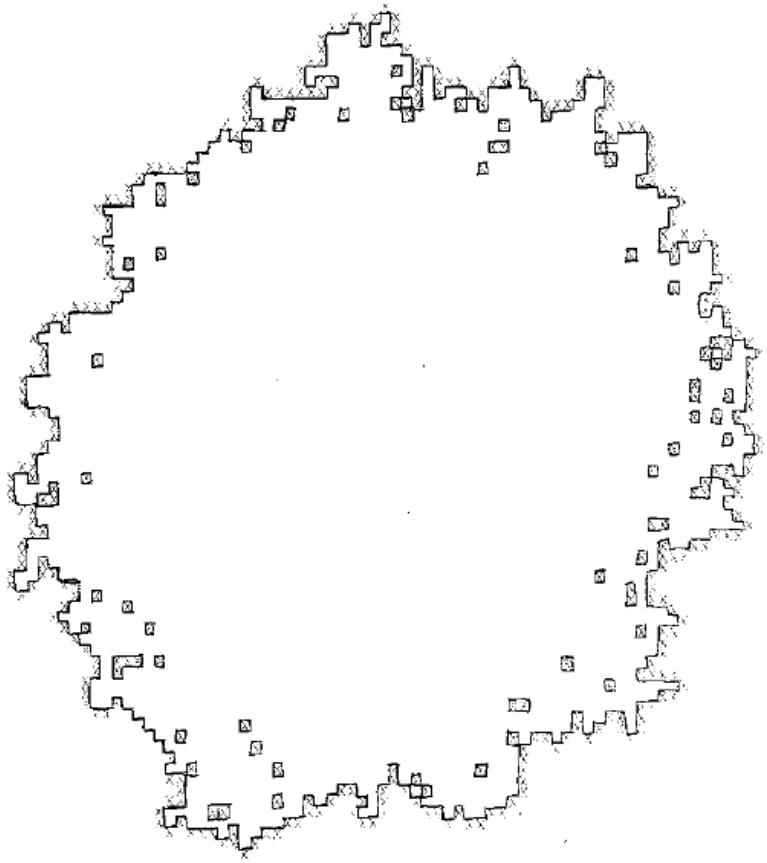
There can be more than one growth site in a column. Can get overhangs.





Eden cluster

ETH

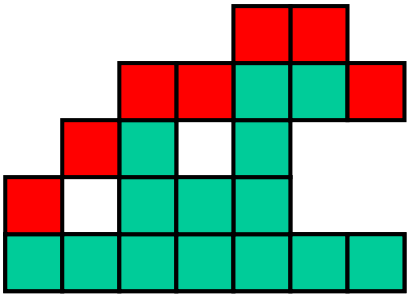


$$\beta = 1/3$$
$$\xi = 1/2$$

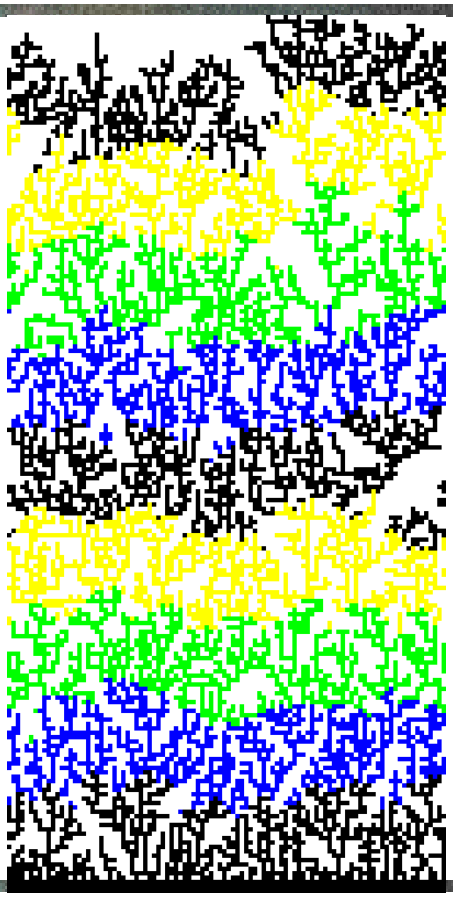
Ballistic deposition

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.



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



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)

$\beta = 1/4$ and $\xi = 1/2$

noise

KPZ equation:

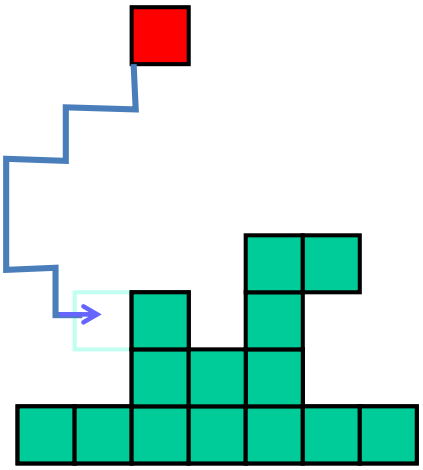
$$\frac{\partial h(x,t)}{\partial t} = \nu \Delta h + \frac{\lambda}{2}(\nabla h)^2 + \eta(x,t)$$

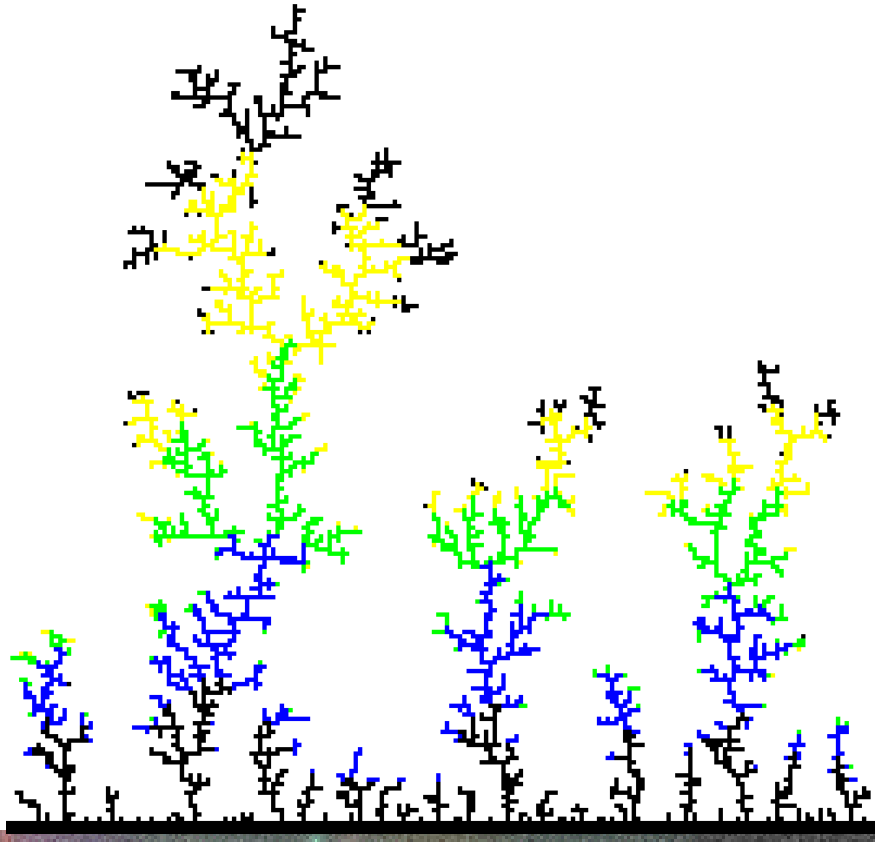
M. Kardar, G. Parisi and Y.-C. Zhang (1986)

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

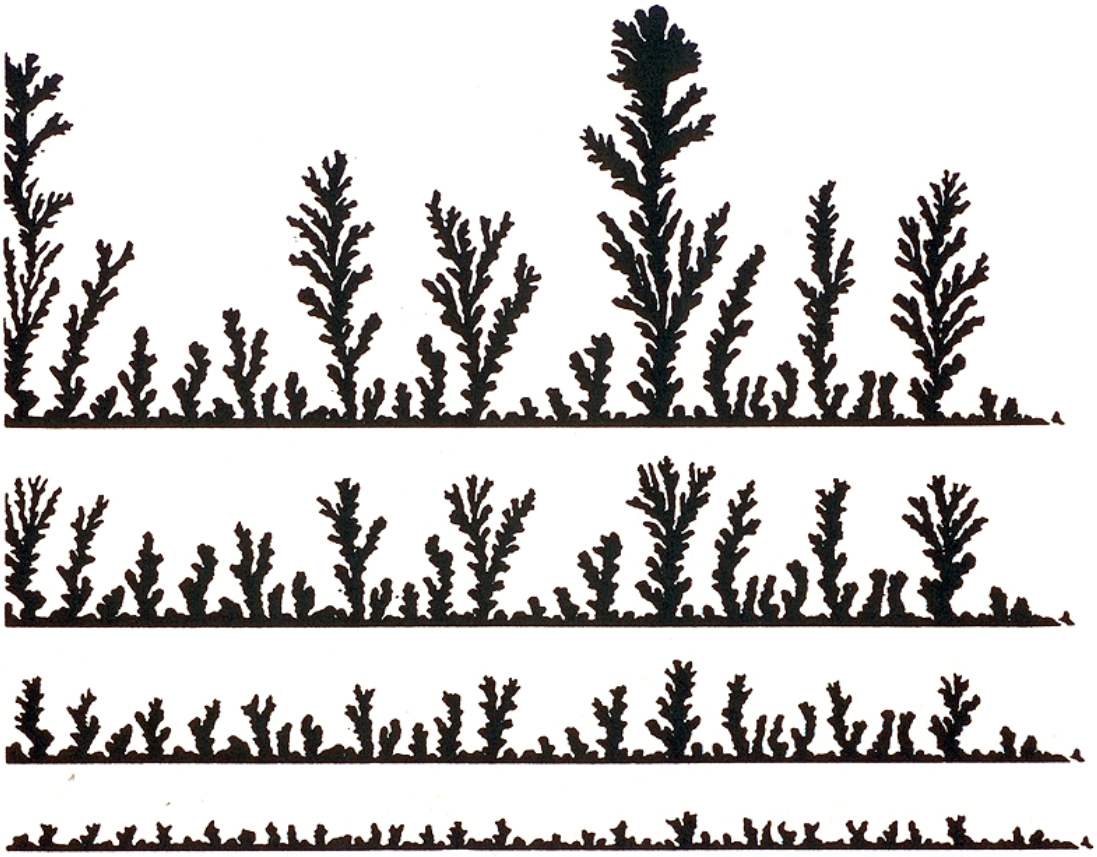
Diffusion Limited Aggregation (DLA)

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

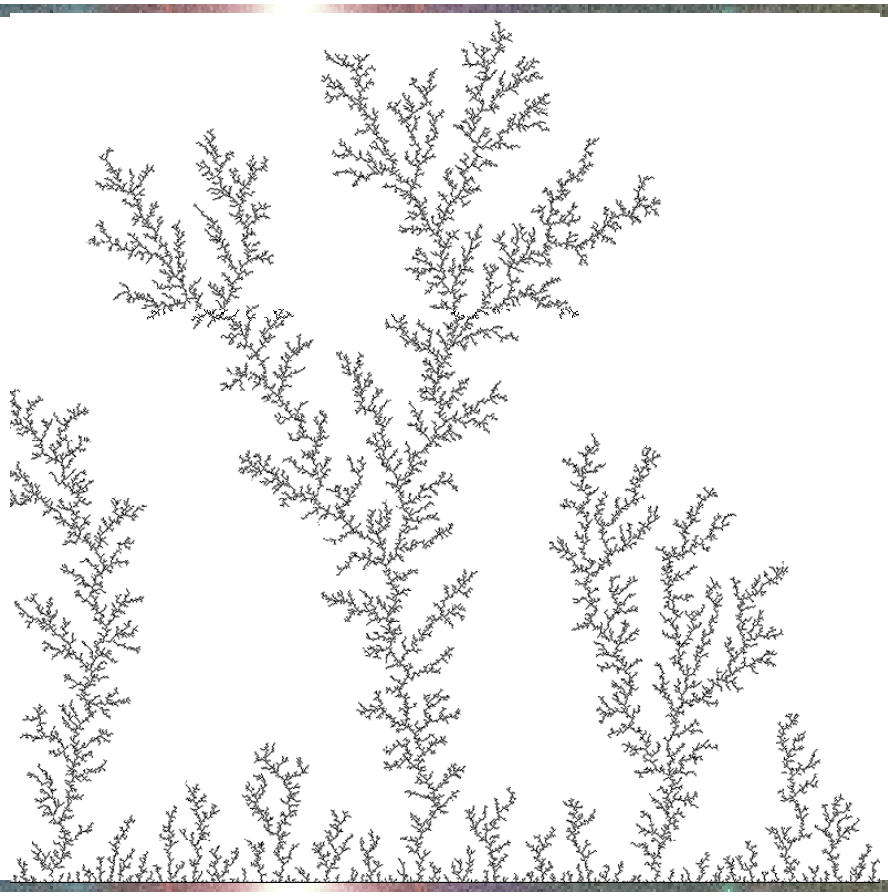




Electrodeposition



DLA clusters

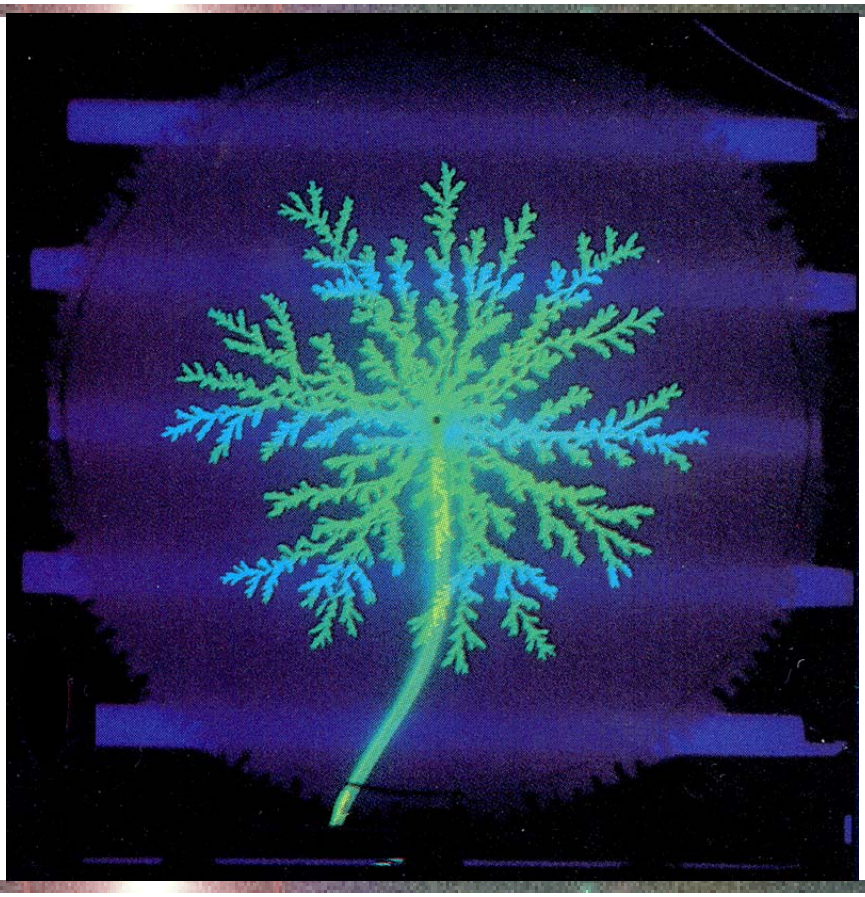


fractal dimension

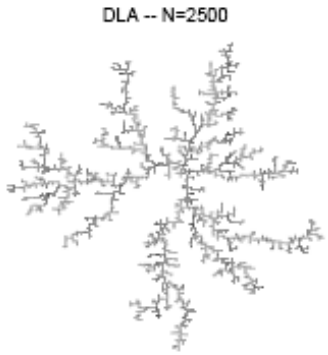
$d_f = 1.7$

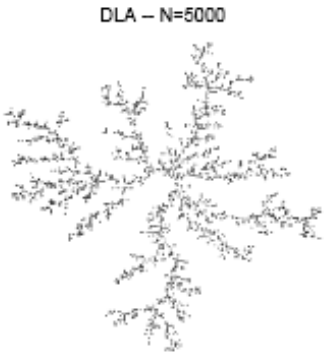
(in 2d)

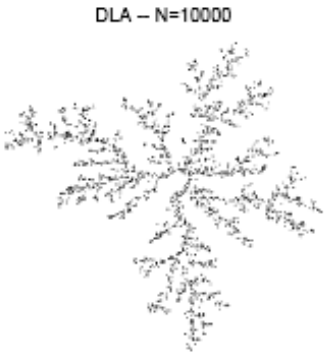
Viscous Fingering

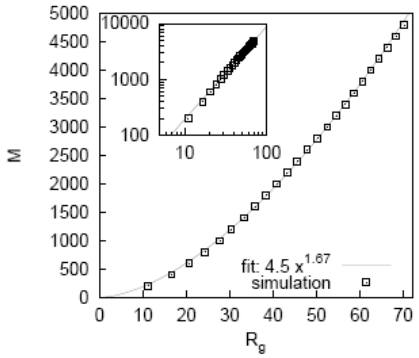


DLA clusters



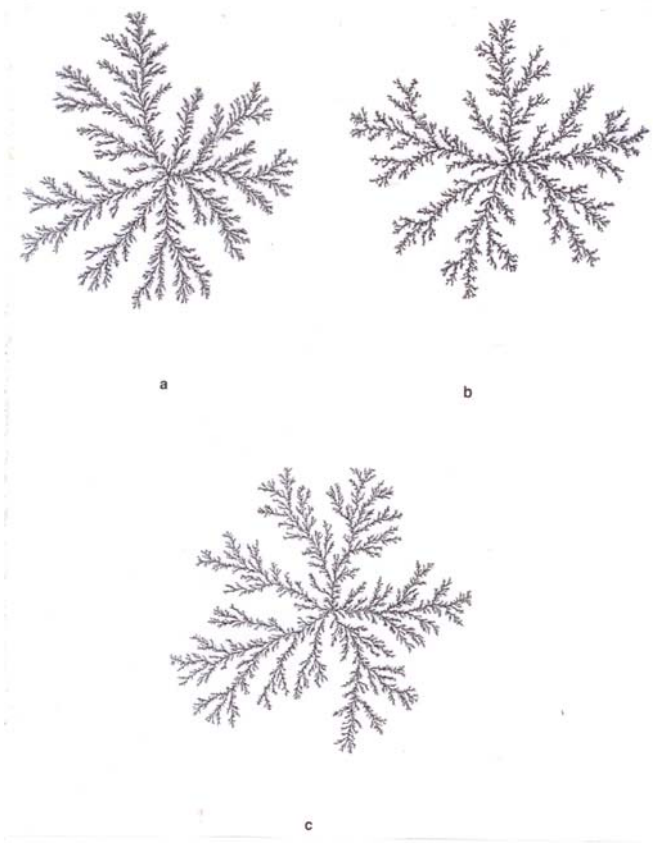




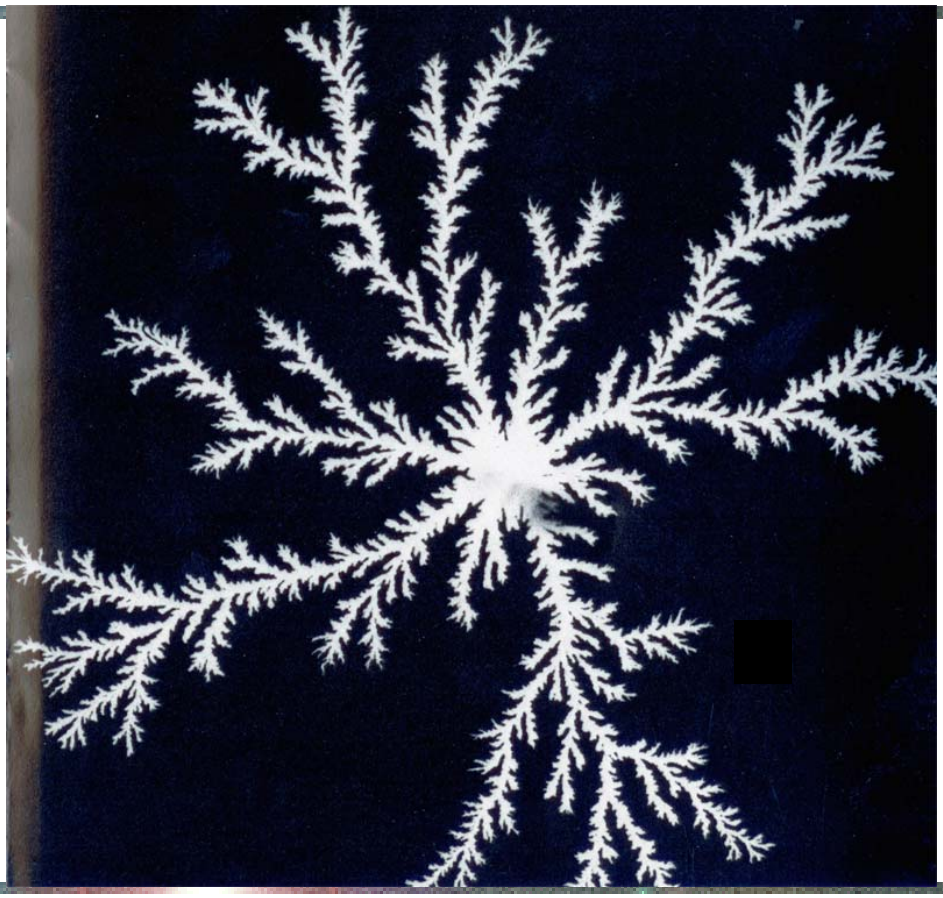


anisotropy on square lattice:

Scale Invariance



Dielectric breakdown



Dielectric breakdown model (DBM)

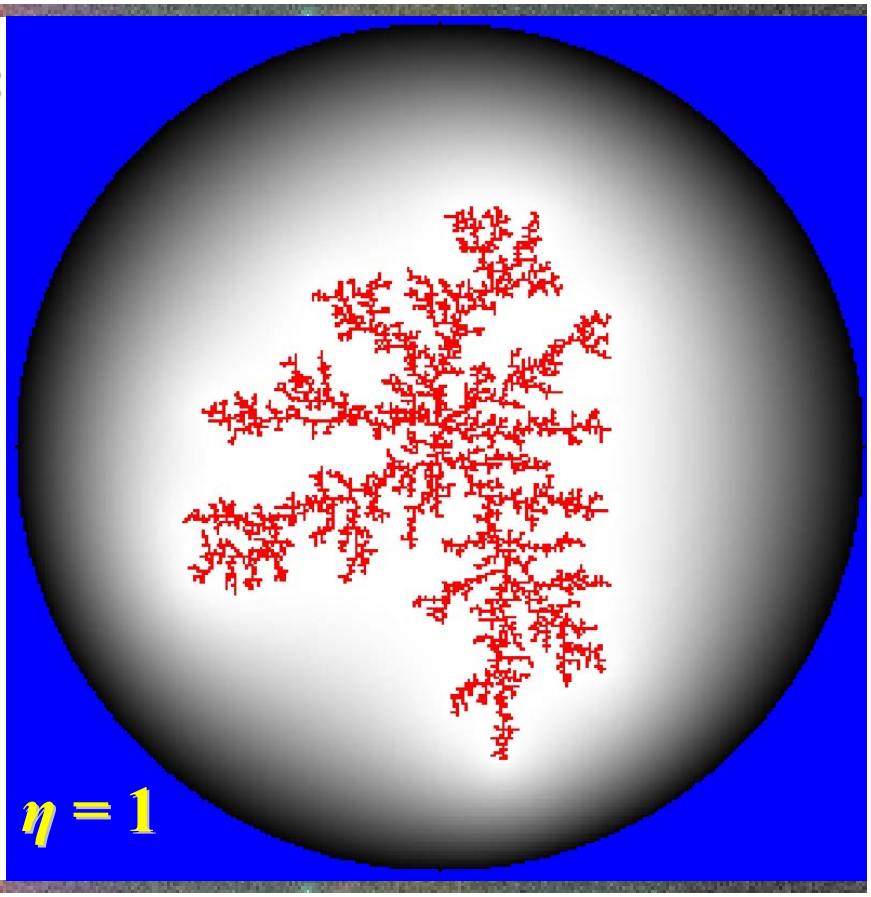
Solve Laplacian field φ:

$$\Delta\phi = 0$$

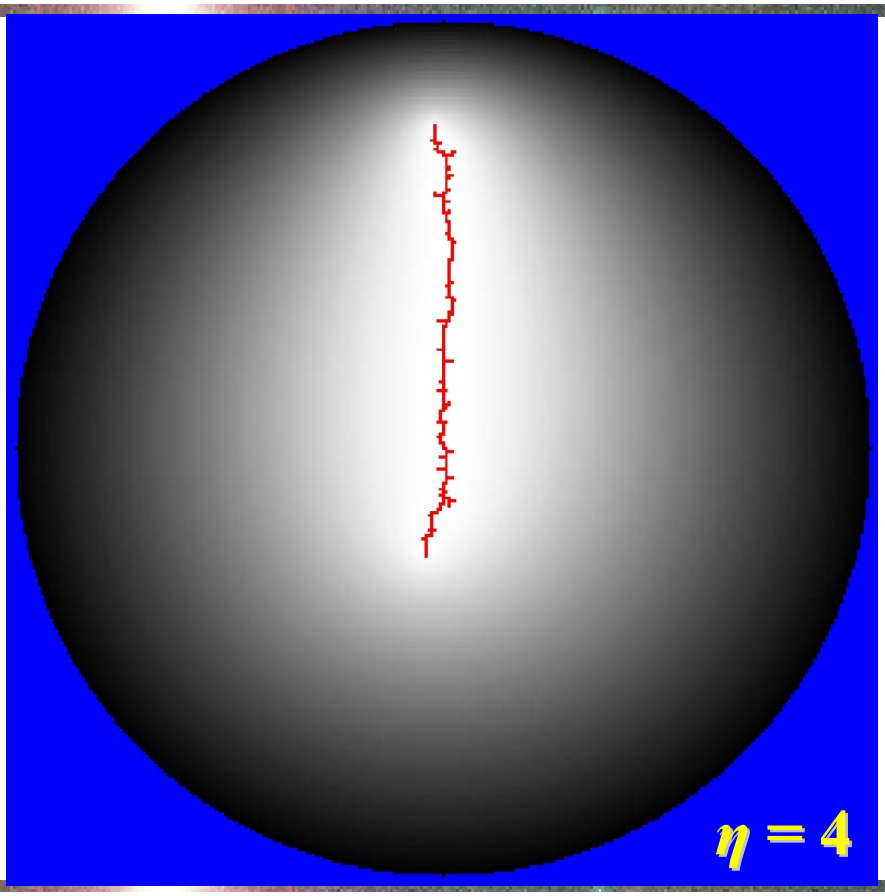
and occupy site at boundary with probability:

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

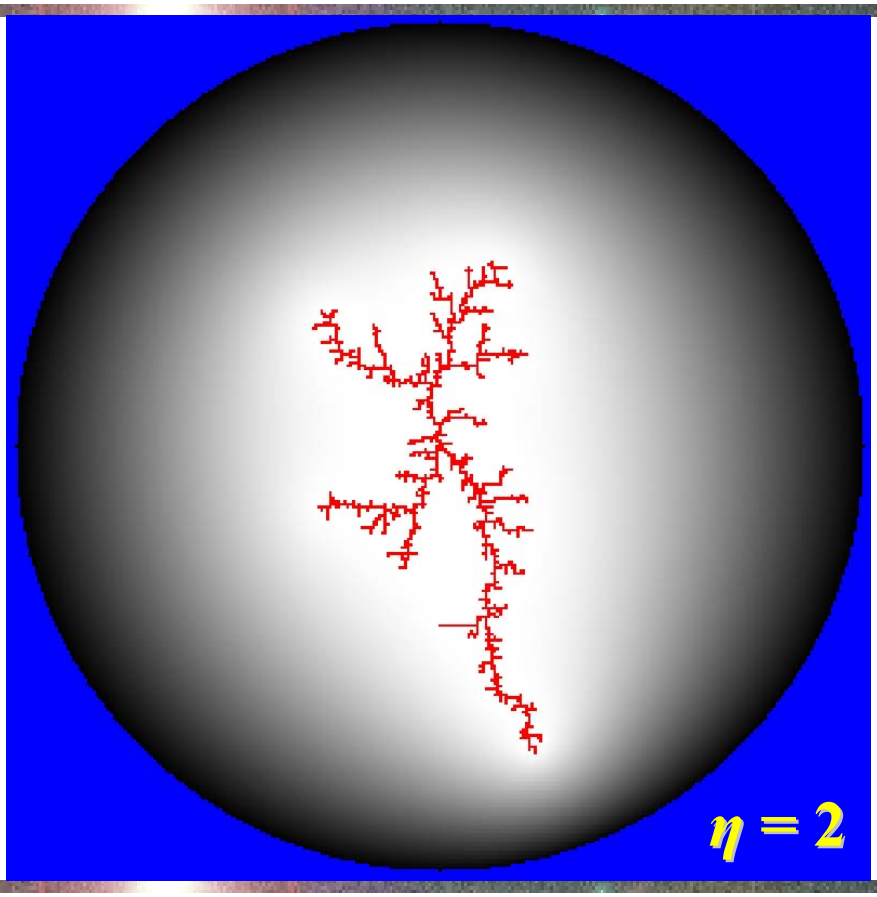
same as DLA



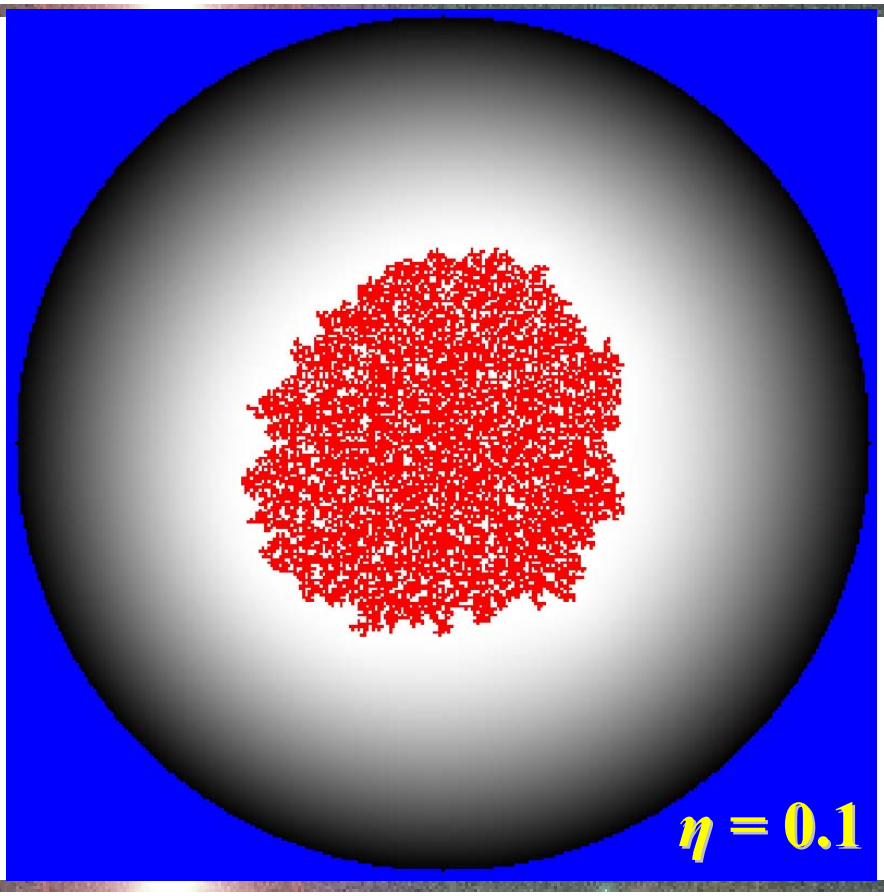
Dielectric breakdown model



Dielectric breakdown model

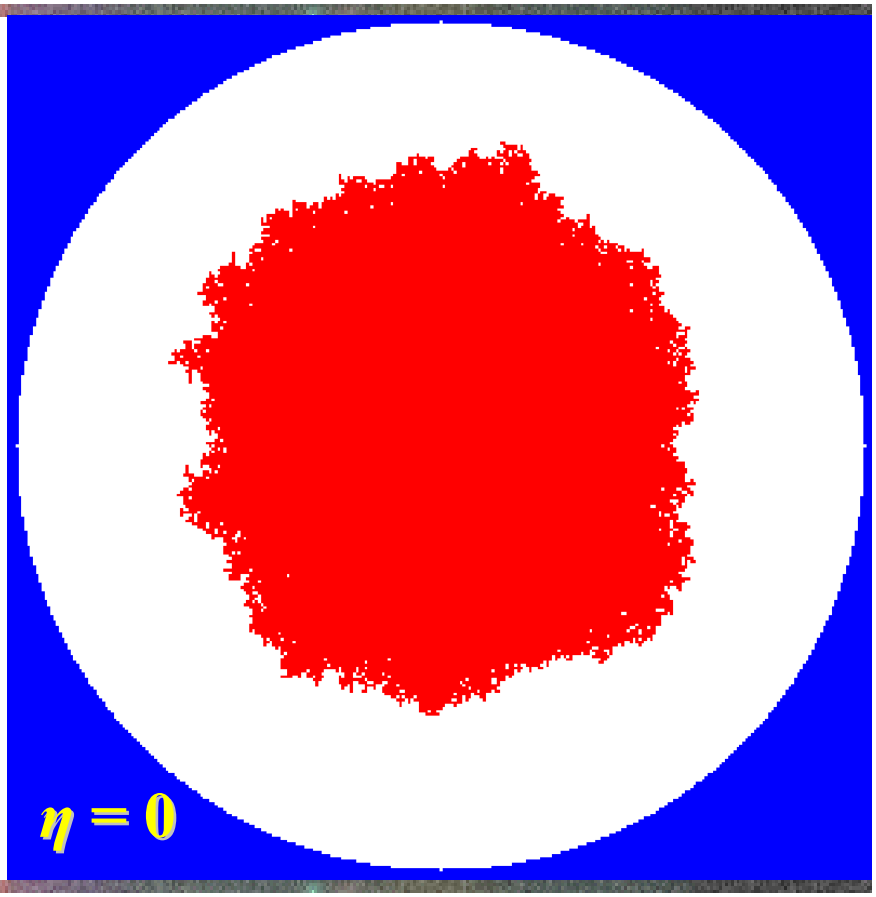


Dielectric breakdown model

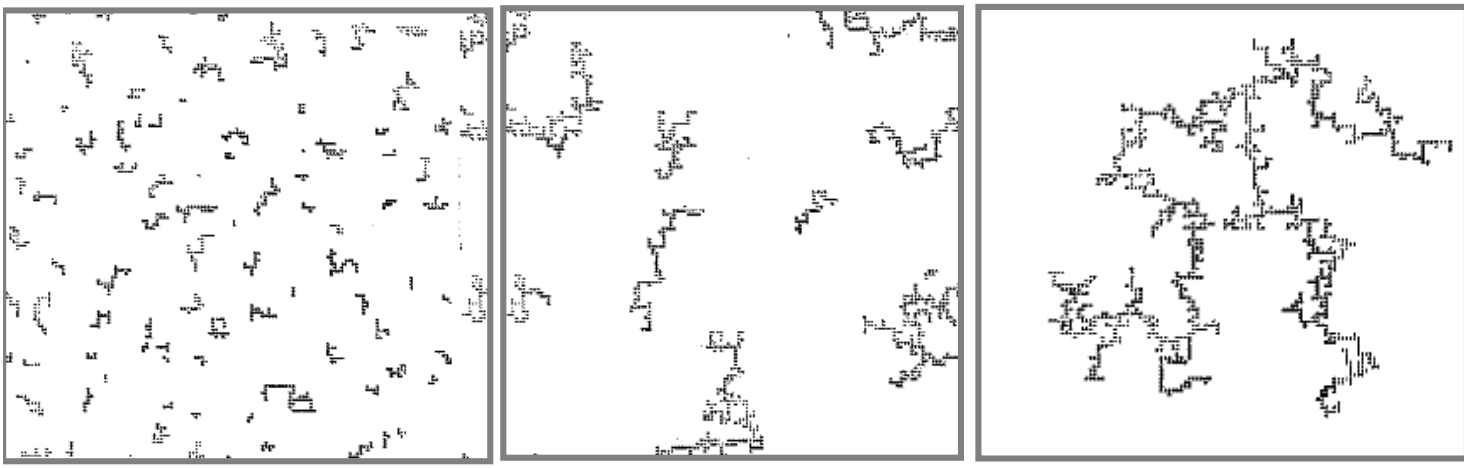


Dielectric breakdown model

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

with dynamical exponent z .

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. Kirckpatrick, 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-complex problem, i.e. time to solve grows faster than any polynomial of n.

Travelling Salesman

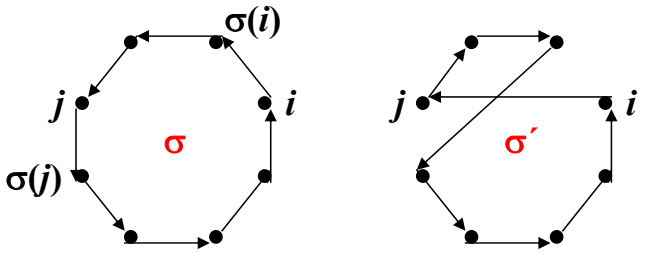
ETH

Make local changes:

$\Rightarrow$ Define close configuration on S

$N : S \rightarrow 2^S$ with $i \in N(j) \Leftrightarrow j \in N(i)$

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



Traditional optimization algorithm:

Improove 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

ETH

Simulated annealing optimization algorithm:

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

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

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

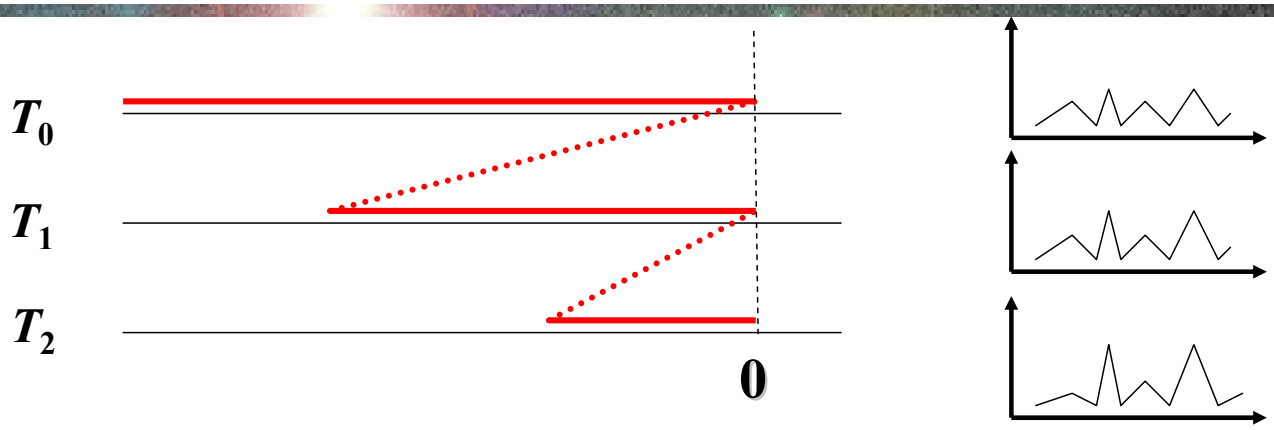
with $\Delta F = F(\sigma') - F(\sigma) > 0$

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.

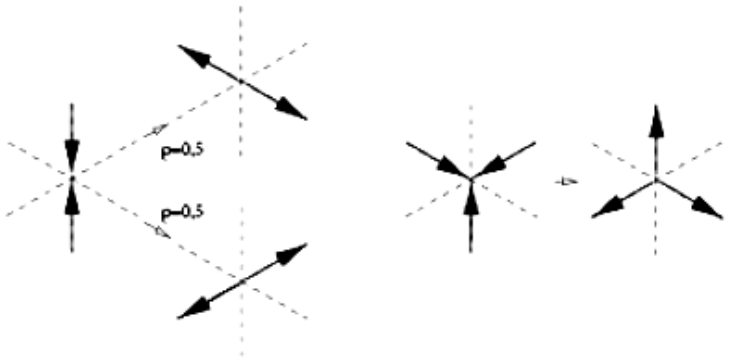
Asymptotic convergence is guarantied and leads to an exponential convergence time.

Lattice gas

- D.H. Rothman and S. Zaleski, „Lattice-Gas Cellular Automata“ (Cambridge Univ. Press, 1997)
- J.-P. Rivet and J.P. Boon, „Lattice Gas Hydrodynamics“ (Cambridge Univ. Press, 2001)
- D.A. Wolf-Gladrow, „Lattice-Gas Cellular Automata and Lattice Boltzmann Models“ (Lecture Notes, Springer, 2000)

Lattice gas

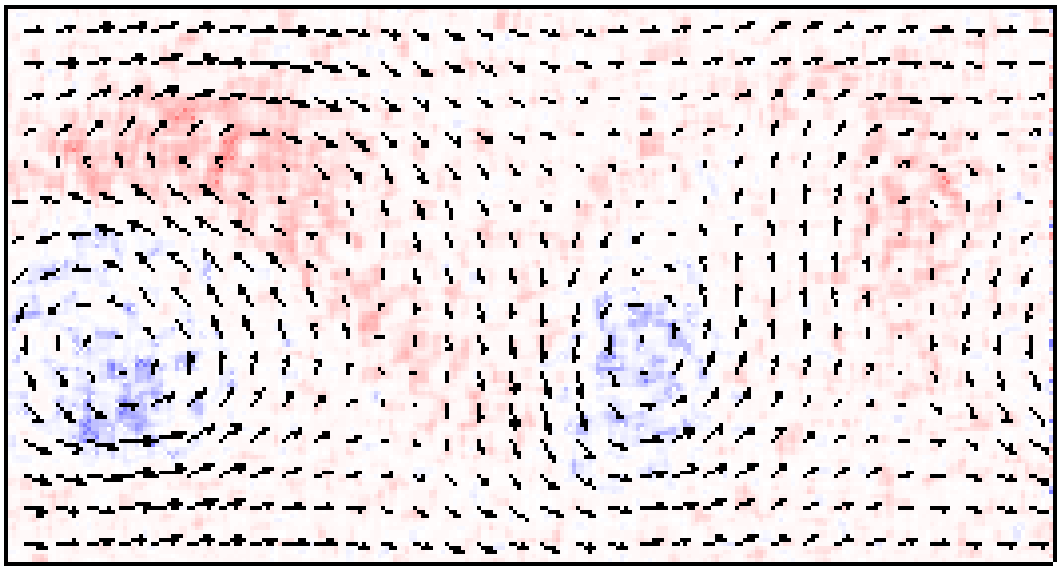
Particles move on a triangular lattice and follow the following collision rules:



Momentum is conserved at each collision.
It can be proven (Chapman-Enskog) that its continuum limit is the Navier Stokes eq.

von Karman street

velocity field of a fluid behind an obstacle



Each vector is an average over time and space.

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:

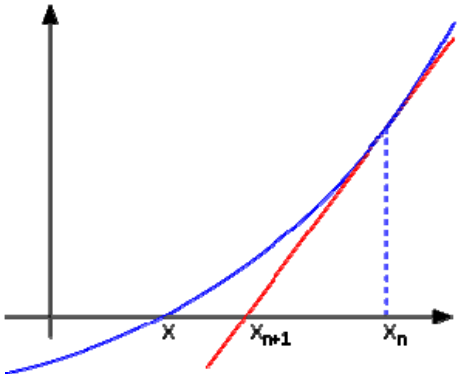
$$\frac{d}{dx} F(x) = 0$$

Newton method

Be x_0 a first guess, then linearize around x_0:

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

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



Secant method

ETH

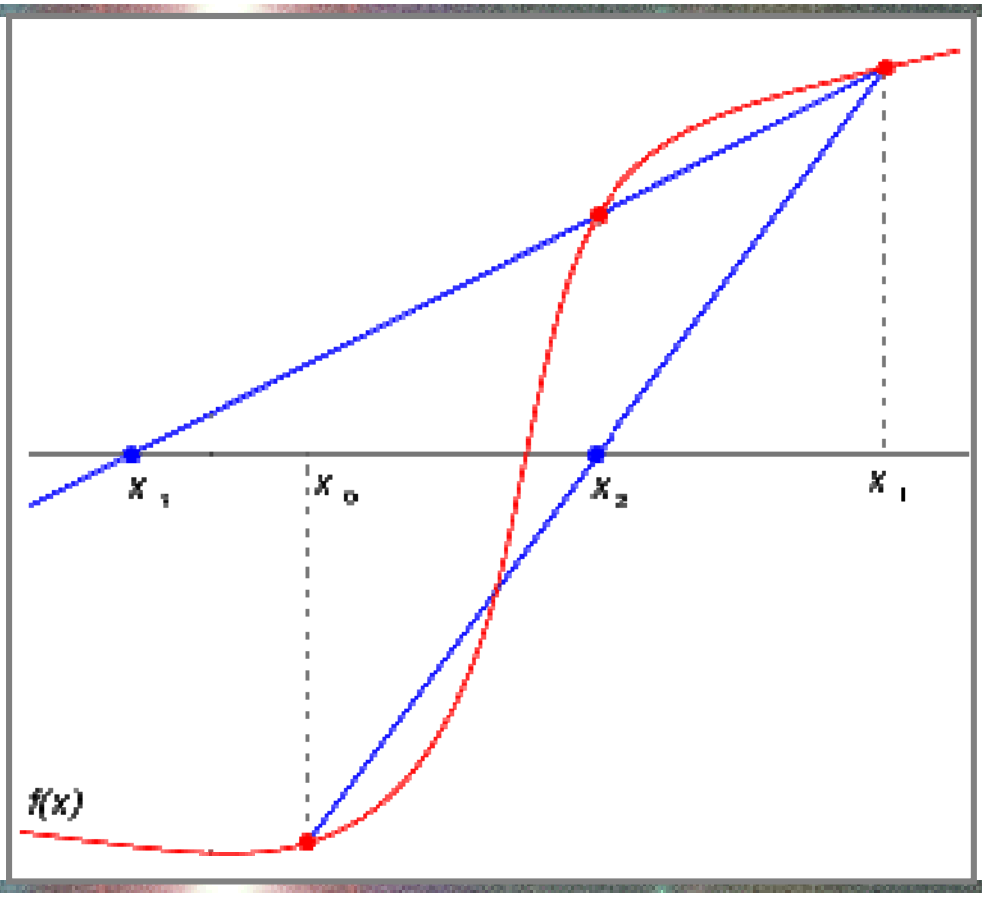
If derivative of *f* is not known analytically:

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

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

Secant method

ETH



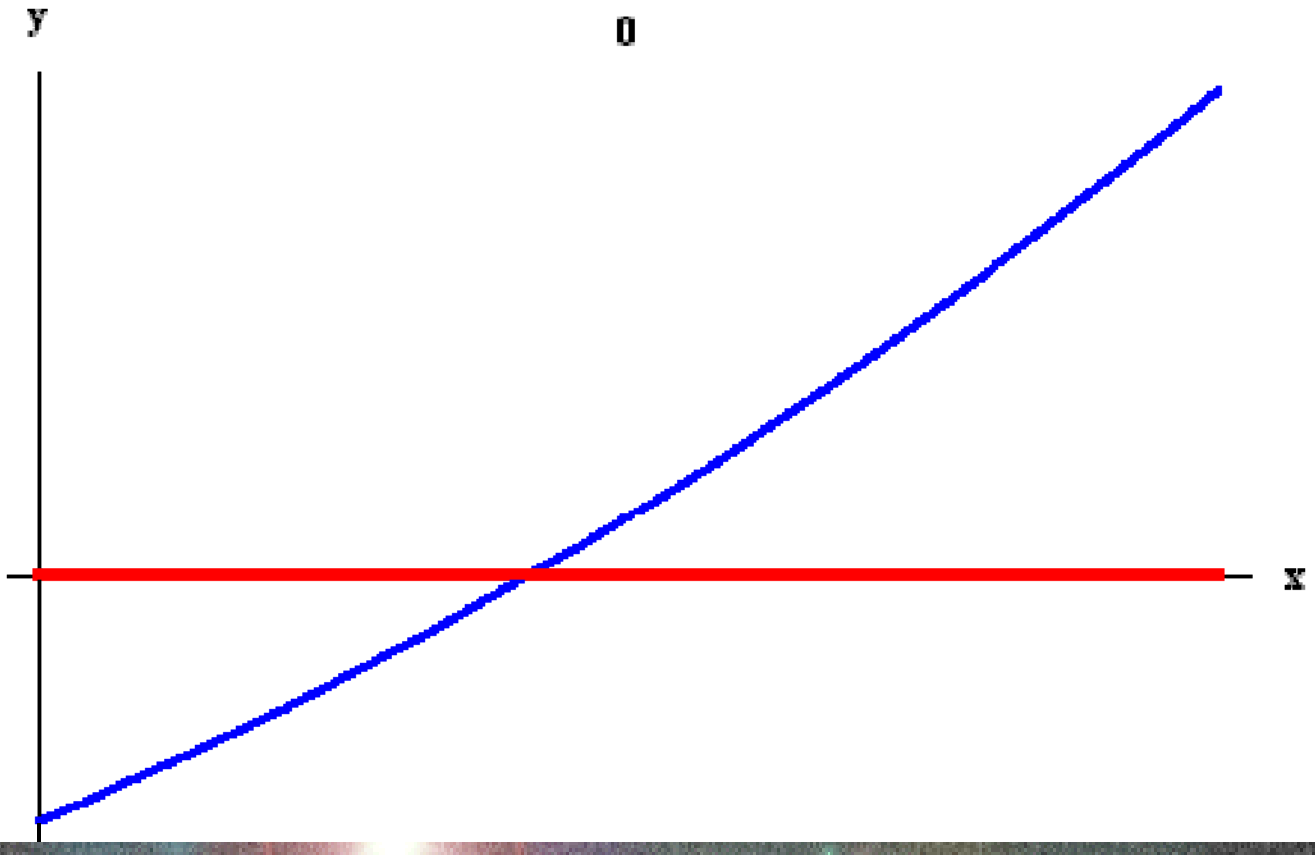
Bisection method

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 sign($f(x_m)$) = sign($f(x_1)$) then replace x_1 by x_m otherwise replace x_2 by x_m.

Bisection method



Regula falsi

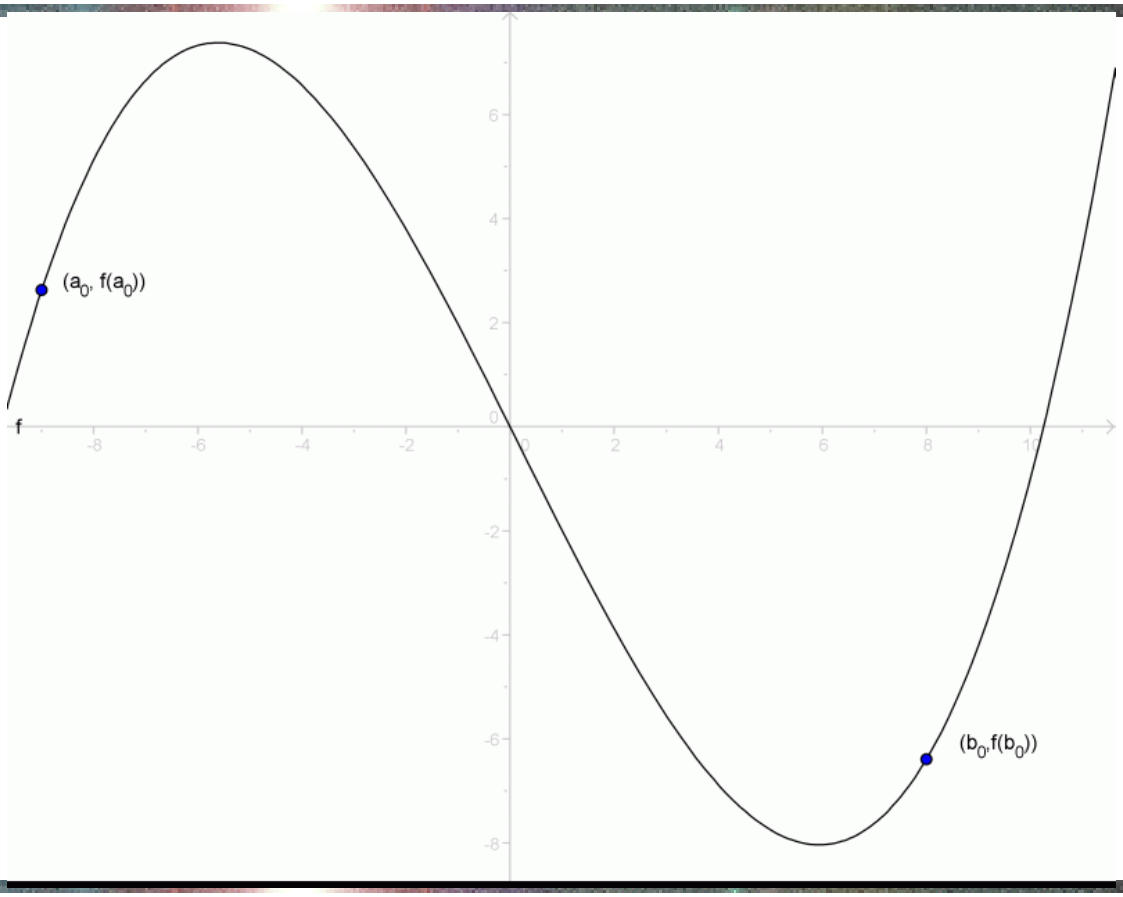
Take two starting values x_1 and x_2 with $f(x_1) < 0$ and $f(x_2) > 0$.

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

Regula falsi



N-dimensional equations

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

System of *N* coupled equations:

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

corresponding to the *N*-dimensional optimization problem:

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

N-dimensional Newton method

Define the Jacobi matrix:

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

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

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

System of linear equations

$$b_{11}x_1 + \ldots + b_{1N}x_N = c_1$$
$$\vdots \qquad\qquad \vdots$$
$$b_{N1}x_1 + \ldots + b_{NN}x_N = c_N$$

$$\Leftrightarrow \vec{\vec{B}}\vec{x} = \vec{c}$$

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

System of linear equations

$$\boxed{\vec{f}(\vec{x}) = \vec{\vec{B}}\vec{x} - \vec{c} = 0 \Rightarrow \vec{\vec{J}} = \vec{\vec{B}}}$$

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

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

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

N-dimensional secant method

ETH

If the derivatives are not known analytically:

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

where h_j should be chosen as:

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

being ε the machine precision,

i.e. $\approx 10^{-16}$ for a 64 bit computer.

Other techniques

ETH

Relaxation method:

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

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:

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

examples:

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

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

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

ETH

Start with y_0 and iterate:

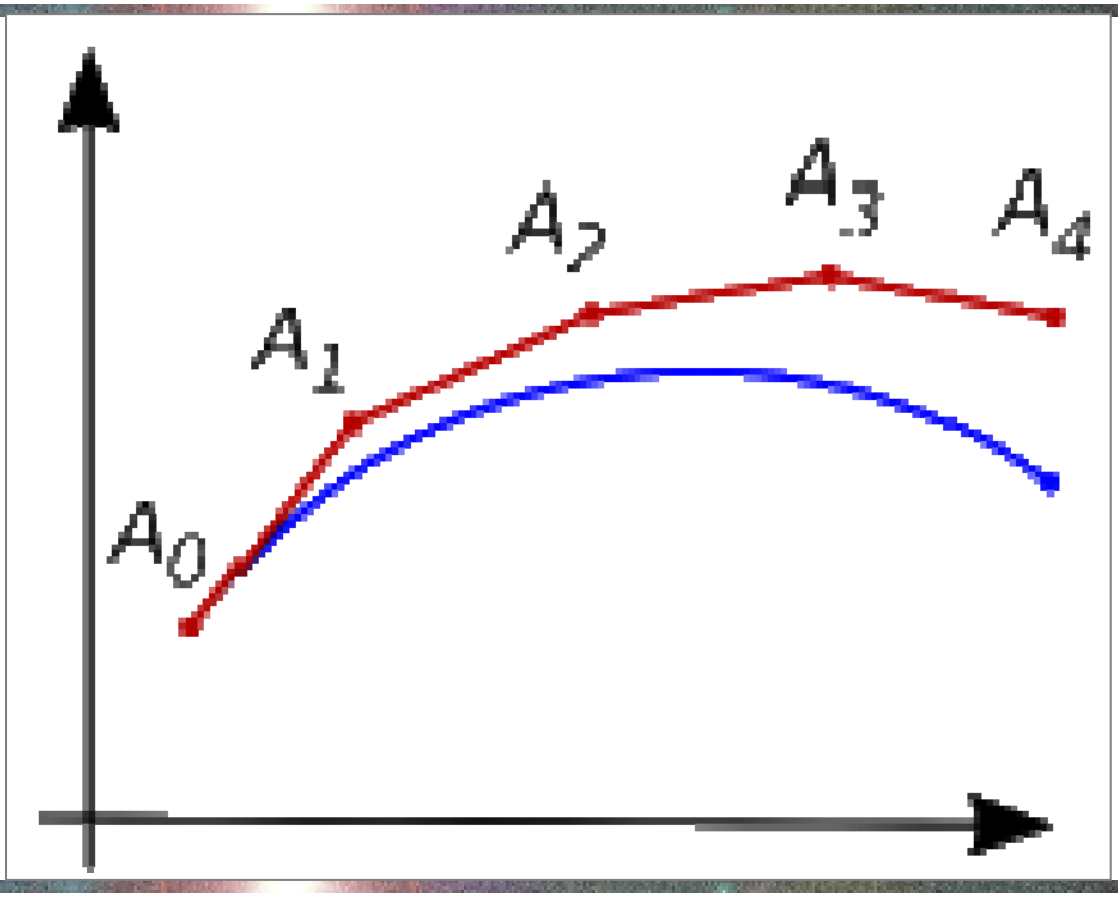
$$y_{n+1} = y_n + \Delta t \cdot f(y_n, t_n) + O(\Delta^2 t)$$

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

ETH



The Newton equation

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

2nd order ODE

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

$$\frac{dx}{dt} = v$$

$$\frac{dv}{dt} = \frac{F(x)}{m}$$

Euler method for *N* coupled ODEs

N coupled ODEs of first order:

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

iterate with a small Δt :

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

with $t_n = t_0 + n \cdot \Delta t$

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:

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

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

The Euler method is globally of first order.

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

Extrapolate using Euler method

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

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

Evaluate derivative in Euler method at this value:

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

Fourth order Runge - Kutta

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

RK4

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

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

ETH

iteration:

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

with

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

and $\alpha_1 = 0$

explicit

implicit:

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

q-stage Runge - Kutta method

ETH

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

Butcher array or Runge-Kutta tableau:

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

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 $p = 4$

applet

Order of Runge - Kutta method

The R-K method is of order p if:

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

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

Taylor expansion:

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

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)

Example: Lorenz equation

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

Warwick Tucker
(2002)

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 $\delta \propto \Delta t^{p+1}$.

Error estimation

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 error as $\delta = y_1 - y_2$

$$y(t+2\Delta t) = \begin{cases} y_1 + (2\Delta t)^{p+1}\Phi + O(\Delta t^{p+2}) \\ y_2 + 2(\Delta t)^{p+1}\Phi + O(\Delta t^{p+2}) \end{cases}$$

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

Error estimation

ETH

improve systematically:

$$y(t+\Delta t) = y_2 + \frac{2\delta}{2^{p+1}-2} + O(\Delta t^{p+2})$$

example RK4:

$$y(t+\Delta t) = y_2 + \frac{\delta}{15} + O(\Delta t^{p+2})$$

Error estimation

ETH

General for two different time steps Δt_1 and Δt_2

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

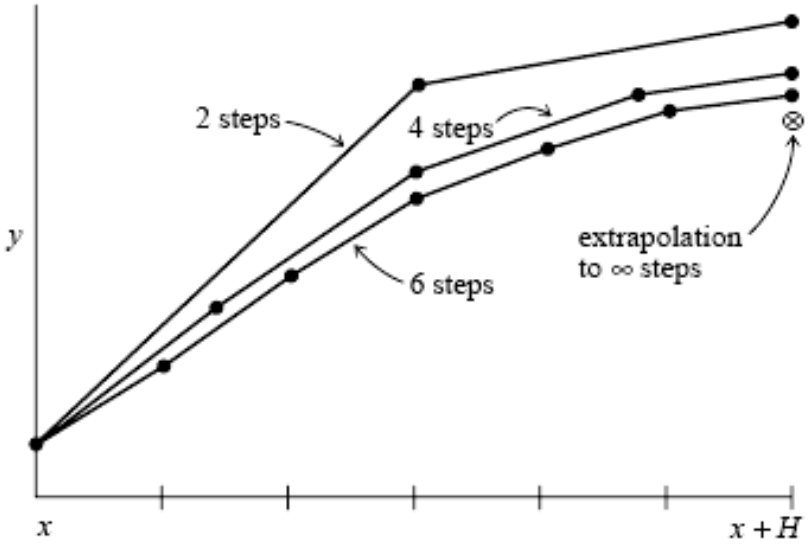
$$\left(\Delta t_2^p - \Delta t_1^p\right) y = \Delta t_2^p y_{\Delta t_1^p} - \Delta t_1^p y_{\Delta t_2^p} + O\left(\Delta t_i^{p+1}\right)$$

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

Richardson extrapolation

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)

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

ETH

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.

Gear coefficients:

$c_0 = 3/8$

$c_2 = 3/4$

$c_3 = 1/6$

5th order predictor- corrector

ETH

Be $r_0 \equiv y$. Then one can define the time derivatives:

$$r_1 = \partial t(dr_0/dt),\ r_2 = 1/2\partial t^2(d^2r_0/dt^2),\ r_3 = 1/6\partial t^3(d^3r_0/dt^3),\ \text{etc.}$$

Predictor:

$$\begin{pmatrix} r_0^p(t+\partial t) \\ r_1^p(t+\partial t) \\ r_2^p(t+\partial t) \\ r_3^p(t+\partial t) \\ r_4^p(t+\partial t) \\ r_5^p(t+\partial t) \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & 2 & 3 & 4 & 5 \\ 0 & 0 & 1 & 3 & 6 & 10 \\ 0 & 0 & 0 & 1 & 4 & 10 \\ 0 & 0 & 0 & 0 & 1 & 5 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} r_0(t) \\ r_1(t) \\ r_2(t) \\ r_3(t) \\ r_4(t) \\ r_5(t) \end{pmatrix}$$

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

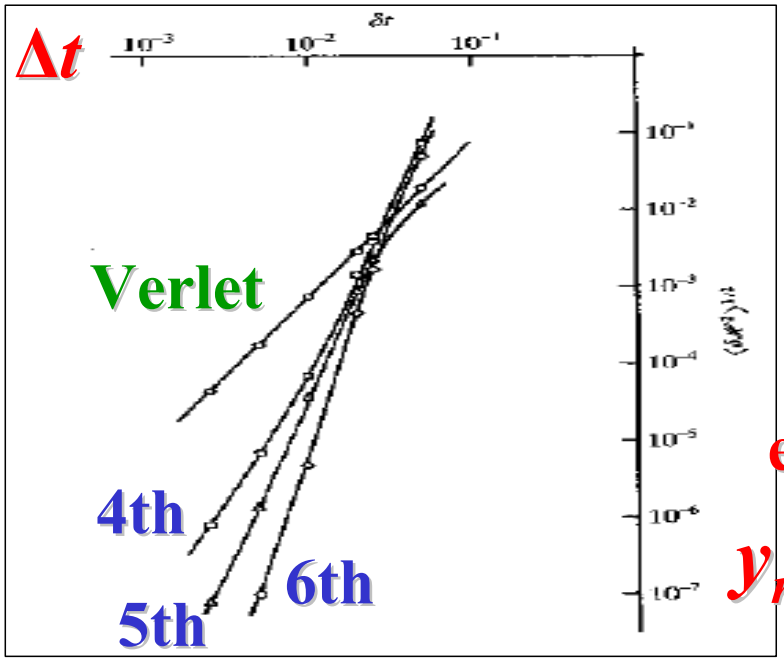
2nd order equation:

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



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:

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

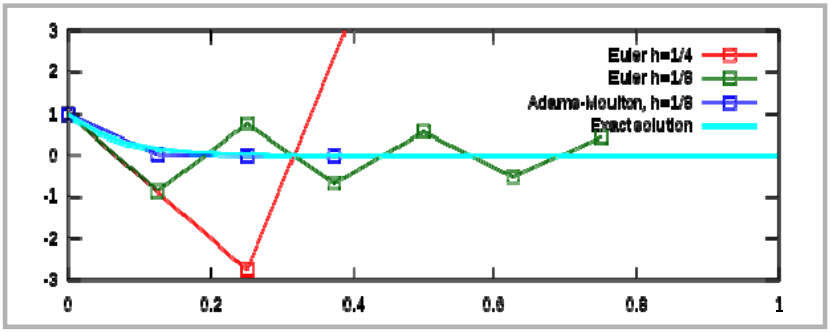
by inserting simultaneously all the values of the previous iteration.

Stiff differential equation

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

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 (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

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

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

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

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

example:

$$y_1' = 998\,y_1 + 1998\,y_2$$
$$y_2' = 999\,y_1 + 1999\,y_2$$
$$y_1(0) = 1 \quad , \quad y_2(0) = 1$$

Solve with with implicit method.