Introduction to Computational Physics

402-0809-00L

Tuesday 10.45 – 12.30 in HPT C 103

Exercises: Tuesday 8.45- 10.30 in HIT F21

Oral exams: end of January

www.ifb.ethz.ch/education/IntroductionComPhys

Studiengänge

- Mathematics, Computer Science (Bachelor)
- Mathematics, Computer Science (Master)
- Physics (Wahlfach)
- Material Science (Master)
- Civil Engineering (Master)

Who is your teacher?

Hans J. Herrmann

hjherrmann@ethz.ch

since April 2006

Institute of Building Materials (IfB)
HIF E12, Hönggerberg, ETH
Zürich

http://comphys.ethz.ch/hans/

Spring term 2010

- **Computational Statistical Physics (H.J.Herrmann)**
- **Computational Quantum Physics (M.Troyer, P.de Forcrand)**
- **Computational Polymer Physics (E. Del Gado)**

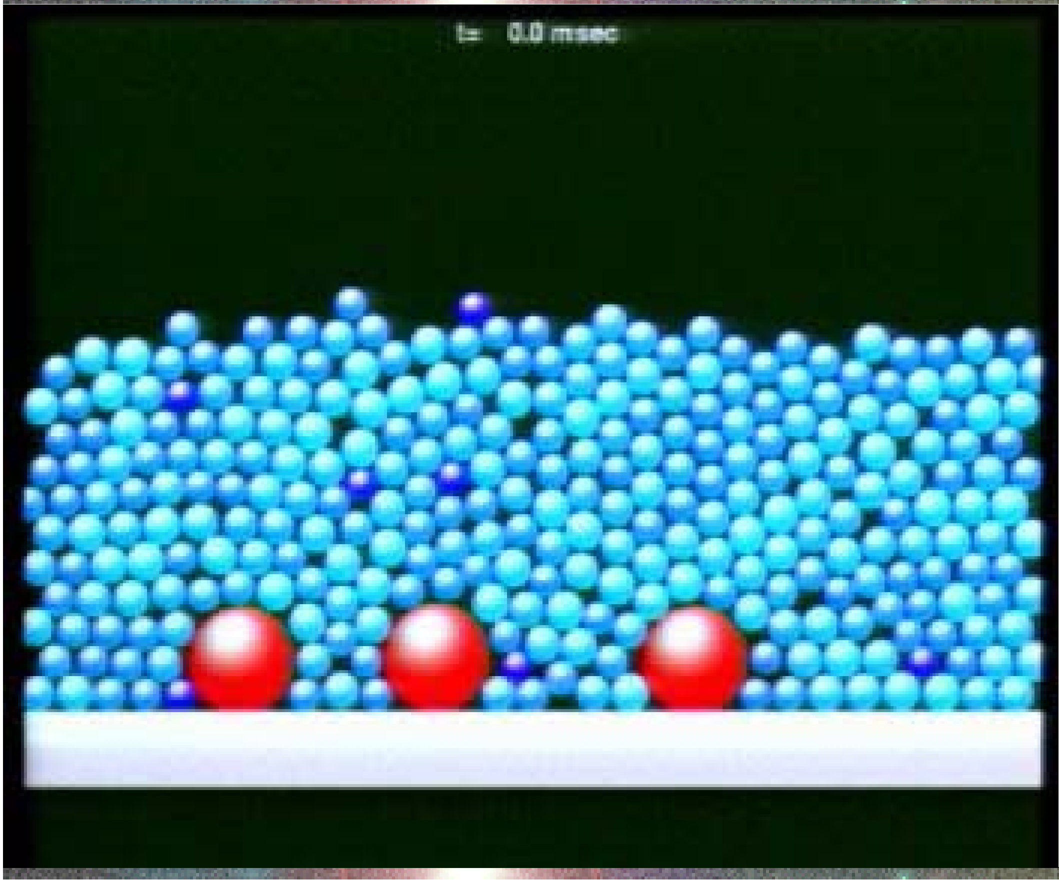
Plan of this course

- 21.09. Introduction, Random numbers (RN)
- 28.09. RN, Percolation
- 05.10. Fractals, Cellular Automata
- 12.10. Ising Model (Troyer)
- 19.10. Random Walks (Del Gado)
- 26.10. Monte Carlo, Importance Sampling, Metropolis
- 02.11. Finite Size Effects, XY Model, first order transitions

Plan of this course

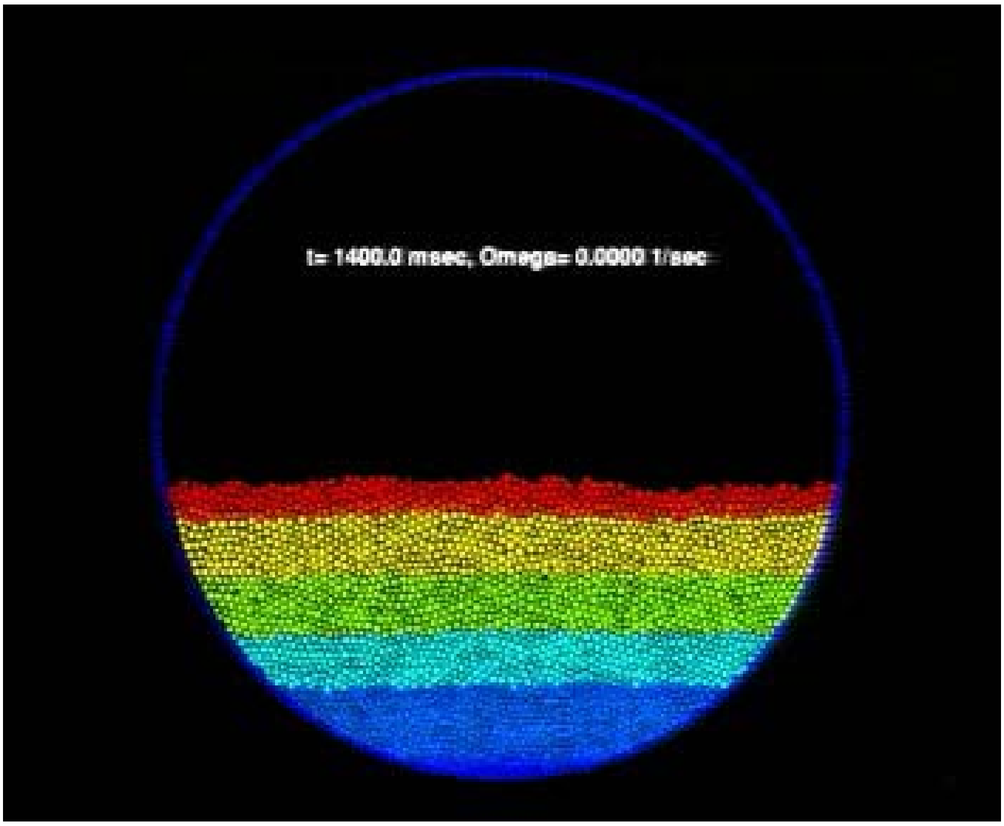
- 09.11. Irreversible Growth, Surfaces
- 16.11. Differential Eqs. (Euler, Runge Kutta..)
- 23.11. Eqs. of Motion (Newton, Regula Falsi)
- 30.11. Finite Difference Meth. Relaxation
- 07.12. Multigrid, Finite Elements Method
- 14.12. Gradient Methods
- 21.12. Variational FEM, Crank-Nicholson Wave equation, Navier-Stokes eq.

Segregation under vibration



Brazil
Nut
Effect

Mixing in a cylinder



hard
spheres

Sedimentation

Glass beads descending in silicon oil

comparing experiment and simulation

Motion of dunes

V. SCHWÄMMLE, H.J. HERRMANN, Nature **426**, 619-620 (2003)

Prerequisites

- Ability to work with UNIX
- Making of Graphical Plots
- Higher computer language (FORTRAN, C++..)
- Statistical Analysis (Averaging, Distributions)
- Linear Algebra, Analysis
- Classical Mechanics
- Basic Thermodynamics

Literature

- H.Gould, J. Tobochnik and W. Christian: „Introduction to Computer Simulation Methods“ 3rd ed. (Wesley, 2006)
- D. Landau and K. Binder: „A Guide to Monte Carlo Simulations in Statistical Physics“ (Cambridge, 2000)
- D. Stauffer, F.W. Hehl, V. Winkelmann and J.G. Zabolitzky: „Computer Simulation and Computer Algebra“ 3rd ed. (Springer, 1993)
- K. Binder and D.W. Heermann: „Monte Carlo Simulation in Statistical Physics“ 4th ed. (Springer, 2002)
- N.J. Giordano: „Computational Physics“ (Wesley, 1996)
- J.M. Thijssen: „Computational Physics“ (Cambridge, 1999)

Book Series

- „Monte Carlo Method in Condensed Matter Physics“, ed. K. Binder (Springer Series)
- „Annual Reviews of Computational Physics“, ed. D. Stauffer (World Scientific)
- „Granada Lectures in Computational Physics“, ed. J.Marro (Springer Series)
- „Computer Simulations Studies in Condensed Matter Physics“, ed. D. Landau (Springer Series)

Journals

- Journal of Computational Physics (Elsevier)
- Computer Physics Communications (Elsevier)
- International Journal of Modern Physics C (World Scientific)

every year (2008: Brazil, 2009 Taiwan, 2010 Trondheim):

CCP = Conference on Computational Physics

What is Computational Physics?

- **Numerical solution of equations** (since analytical solutions are rare)
- **Simulation of many-particle systems** (creation of a virtual reality = 3rd branch of physics)
- **Evaluation and visualization of large data sets** (either experimental or numerical)
- **Control of experiments** (not treated in this course)

Areas of computational physics

- CFD (Computational Fluid Dynamics)
- Classical Phase Transitions
- Solid State (quantum)
- High Energy Physics (Lattice QCD)
- Astrophysics
- Geophysics, Solid Mechanics
- Agent models (interdisciplinary)

Computer tools

- **Object oriented programming**
- **Vector supercomputers**
- **Parallel computing (shared and distributed memory)**
- **Symbolic Algebra (Mathematica, Maple)**
- **Graphical animations**

Random numbers

10480	15011	01536	02011	81647	91646	69179	14194	62590
22368	46573	25595	85393	30995	89198	27982	53402	93965
24130	48360	22527	97265	76393	64809	15179	24830	49340
42167	93093	06243	61680	07856	16376	39440	53537	71341
37570	39975	81837	16656	06121	91782	60468	81305	49684
77921	06907	11008	42751	27756	53498	18602	70659	90655
99562	72905	56420	69994	98872	31016	71194	18738	44013
96301	91977	05463	07972	18876	20922	94595	56869	69014
89579	14342	63661	10281	17453	18103	57740	84378	25331
85475	36857	53342	53988	53060	59533	38867	62300	08158
28918	69578	88231	33276	70997	79936	56865	05859	90106
63553	40961	48235	03427	49626	69445	18663	72695	52180
09429	93969	52636	92737	88974	33488	36320	17617	30015
10365	61129	87529	85689	48237	52267	67689	93394	01511
07119	97336	71048	08178	77233	13916	47564	81056	97735
51085	12765	51821	51259	77452	16308	60756	92144	49442
02368	21382	52404	60268	89368	19885	55322	44819	01188
01011	54092	33362	94904	31273	04146	18594	29852	71585
52162	53916	46369	58586	23216	14513	83149	98736	23495
07056	97628	33787	09998	42698	06691	76988	13602	51851
48663	91245	85828	14346	09172	30168	90229	04734	59193
54164	58492	22421	74103	47070	25306	76468	26384	58151
32639	32363	05597	24200	13363	38005	94342	28728	35806
29334	27001	87637	87308	58731	00256	45834	15398	46557
02488	33062	28834	07351	19731	92420	60952	61280	50001
81525	72295	04839	96423	24878	82651	66566	14778	76797
29676	20591	68086	26432	46901	20849	89768	81536	86645
00742	57392	39064	66432	84673	40027	32832	61362	98947
05366	04213	25669	26422	44407	44048	37937	63904	45766
91921	26418	64117	94305	26766	25940	39972	22209	71500
00582	04711	87917	77341	42206	35126	74087	99547	81817
00725	69884	62797	56170	86324	88072	76222	36086	84637
69011	65795	95876	55293	18988	27354	26575	08625	40801
25976	57948	29888	88604	67917	48708	18912	82271	65424
09763	83473	73577	12908	30883	18317	28290	35797	05998
91567	42595	27958	30134	04024	86385	29880	99730	55536
17955	56349	90999	49127	20044	59931	06115	20542	18059
46503	18584	18845	49618	02304	51038	20655	58727	28168
92157	89634	94824	78171	84610	82834	09922	25417	44137
14577	62765	35605	81263	39667	47358	56873	56307	61607
98427	07523	33362	64270	01638	92477	66969	98420	04880
34914	63976	88720	82765	34476	17032	87589	40836	32427
70060	28277	39475	46473	23219	53416	94970	25832	69975
53976	54914	06990	67245	68350	82948	11398	42878	80287
76072	29515	40980	07391	58745	25774	22987	80059	39911
90725	52210	83974	29992	65831	38857	50490	83765	55657
64364	67412	33339	31926	14883	24413	59744	92351	97473
08962	00358	31662	25388	61642	34072	81249	35648	56891
95012	68379	93526	70765	10592	04542	76463	54328	02349
15664	10493	20492	38391	91132	21999	59516	81652	27195

Why do we need Random numbers?

- **Simulate experimental fluctuations** (e.g. radioactive decay)
- **Define temperature**
- **Complement lack of detailed knowledge** (e.g. traffic or stock market simulations)
- **Consider many degrees of freedom** (e.g. Bownian motion)
- **Test stability to perturbations**
- **Random sampling**

Literature to Random numbers

- **Numerical Recipes**
- **D.E.Knuth: „ The Art of Programming: Seminumerical Algorithms“ 3rd ed. (Addison – Wesley, 1997) Vol. 2, Chapt. 3.3.1**
- **J.E. Gentle, „Random Number Generation and Monte Carlo Methods“ (Springer, 2003)**

Properties of Random numbers

- No correlations
- Long periods
- Follow well-defined distribution
- Fast implementation
- Reproductibility

Distribution of random numbers

$$\int_{-\infty}^{+\infty} P(x)dx = 1 \quad \text{and} \quad P(x) > 0$$

examples: homogeneous, Gaussian, Poisson

Probability to find a random number in the interval [x, $x + \Delta x$]:

$$w(x) = \int_{x}^{x+\Delta x} P(x)dx$$

Random number generators (RNG)

electrical flicker noise

photon emission
from a semiconductor

Algorithms:

- **Congruential** (Lehmer, 1948)
- **Lagged-Fibonacci** (Tausworth,1965)

Congruential generators

Fix two integers: c and p .

Start with a **seed** x_0 .

Create new integers by iterating :

$$\boxed{x_i = (c \cdot x_{i-1}) \bmod p \quad , \qquad x_i, c, p \in \mathbb{Z}}$$

Make random numbers $\boxed{z_i \in [0,1)}$

through $$\boxed{z_i = \frac{x_i}{p}}$$

Maximal period

Since all integers are less than p the sequence must repeat after at least p -1 iterations, i.e. the maximal period is p -1.

($x_0 = 0$ is a fixed point and cannot be used.)

R.D. Carmichael proved 1910 that one gets the maximal period if p is a Mersenne prime number and the smallest integer number for which

$$c^{p-1} \bmod p = 1$$

Robert D. Carmichael

Mersenne prime numbers

$$M_q = 2^q - 1$$

q prime

Marin Mersenne, 1626

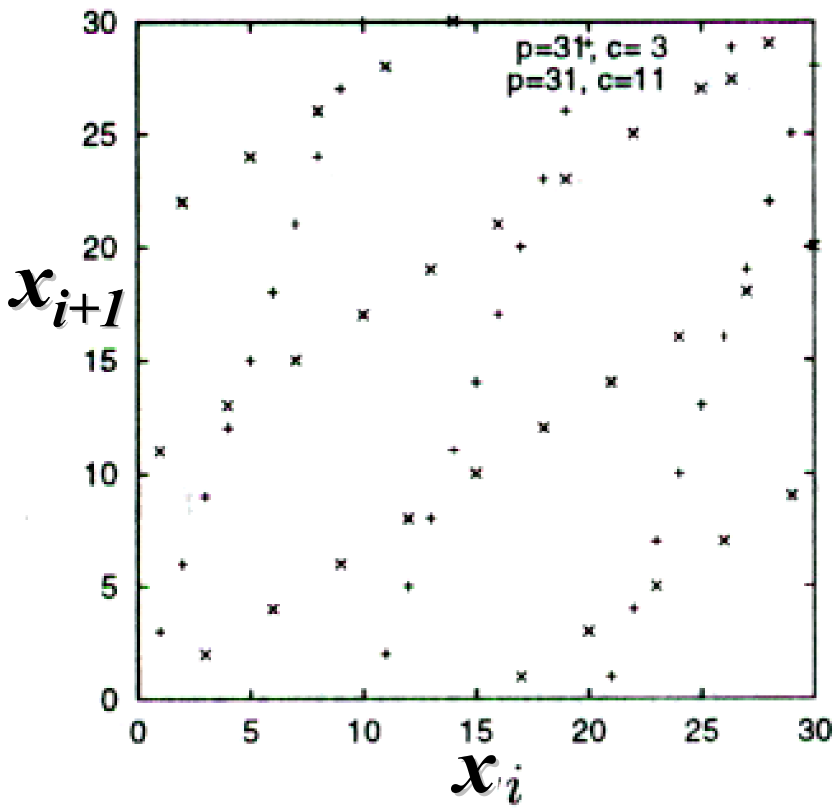
	n	M_n	Digits in M_n	Date of discovery	Discover
1	2	3	1	*ancient*	*ancient*
2	3	7	1	*ancient*	*ancient*
3	5	31	2	*ancient*	*ancient*
4	7	127	3	*ancient*	*ancient*
5	13	8191	4	1456	*anonymous* [4]
6	17	131071	6	1588	Cataldi
7	19	524287	6	1588	Cataldi
8	31	2147483647	10	1772	Euler
9	61	2305843009213693951	19	1883	Pervushin
43*	30,402,457	315416475…652943871	9,152,052	December 15, 2005	GIMPS / Curtis & Steven Boon
44*	32,582,657	124575026…053967871	9,808,358	September 4, 2006	GIMPS / Curtis & Steven Boon

Example of congruential RNG

Park and Miller (1988):

```
const int p=2147483647;
const int c=16807;
int rnd=42;  //seed
rnd = (c*rnd) % p;
print rnd;
```


Square test



Applet

Theorem of Marsaglia

Marsaglia (1968)

For a congruential generator the random numbers in an *n*-cube-test lie on parallel *n* -1 dimensional hyperplanes.

$$\exists\, a_1, \ldots, a_n : \; (a_1 x_i + a_2 x_{i+1} + \ldots + a_n x_{i+n-1}) \bmod p = 0$$

proof using:

$\exists \forall p, c, n$ at least one set $a_1, \ldots, a_n$:

$$\left(a_1 c^1 + \ldots + a_n c^n\right) \bmod p = 0$$

n-cube-test

One can also show that for congruential RNG the distance between the planes must be larger than

$$\sqrt{\frac{p}{n}}$$

and that the maximum number of planes is

$$p^{1/n}$$

Lagged-Fibonacci RNG

- Initialization of *b* random **bits** x_i
- Apply:

$$x_i = \left(\sum_{j \in \Im} x_{i-j}\right) \bmod 2$$

$$\Im \subset [1,..,b]$$

Lagged Fibbonacci RNG

Typically one uses, since it is easy to implement:

$$\boldsymbol{x}_i = \boldsymbol{x}_{i-a} \oplus \boldsymbol{x}_{i-b} \equiv \left(\boldsymbol{x}_{i-a} + \boldsymbol{x}_{i-b}\right) \bmod 2$$

$$\boldsymbol{a} < \boldsymbol{b}$$

Theorem of A. Compagner (1992) :

If (*a*,*b*) Zierler trinomial then sequence has maximal period $2^b - 1$ and :

$$\langle \boldsymbol{x}_i \cdot \boldsymbol{x}_{i-k} \rangle - \langle \boldsymbol{x}_i \rangle^2 = 0 \qquad \forall\ \boldsymbol{k} < \boldsymbol{b}$$

Zierler trinomials

$$\boxed{1 + x^a + x^b}$$

primitive on $Z_2[x]$
(Zierler, 1969)

(a, b)

(103, 250) (Kirkpatrick and Stoll, 1981)

(1689, 4187)

(54454, 132049) (J.R. Heringa et al., 1992)

(3037958, 6972592) (R.P.Brent et al., 2003)

Making 64-bit integers

.....

z_i = (01101....101110)

z_{i+1} = (10001....010111)

z_{i+2} = (00101....111001)

z_{i+3} = (01011....011100)

z_{i+4} = (00011....011011)

.....

Tests for random numbers

- Check distribution
- Average is 0.5
- Average of each bit is 0.5
- *n*-cube-test
- Correlations should vanish
- Spectral test: no peaks in Fourier transform
- $\chi 2$ test: partial sums follow a Gaussian
- Kolmogorov – Smirnov test

→ „Diehard battery" of Marsaglia (1995)

Diehard battery

- **Birthday Spacings**: Choose random points on a large interval. The spacings between the points should be Poisson distributed.
- **Overlapping Permutations**: Analyze sequences of five consecutive random numbers. The 120 possible orderings should occur with statistically equal probability.
- **Ranks of matrices**: Select some number of bits from some number of random numbers to form a matrix over {0,1}, then determine the rank of the matrix. Count the ranks.
- **Monkey Tests**: Treat sequences of some number of bits as "words". Count the overlapping words in a stream. The number of "words" that don't appear should follow a known distribution.
- **Count the 1s**: Count the 1 bits in each of either successive or chosen bytes. Convert the counts to "letters", and count the occurrences of five-letter "words".
- **Parking Lot Test**: Randomly place unit circles in a 100 x 100 square. If the circle overlaps an existing one, try again. After 12,000 tries, the number of successfully "parked" circles should follow a normal distribution.
- **Minimum Distance Test**: Randomly place 8,000 points in a 10,000 x 10,000 square, then find the minimum distance between the pairs. The square of this distance should be exponentially distributed.
- **Random Spheres Test**: Randomly choose 4,000 points in a cube of edge 1,000. Center a sphere on each point, whose radius is the minimum distance to another point. The smallest sphere's volume should be exponentially distributed with a certain mean.
- **The Squeeze Test**: Multiply 231 by random floats on [0,1) until you reach 1. Repeat this 100,000 times. The number of floats needed to reach 1 should follow a certain distribution.
- **Overlapping Sums Test**: Generate a long sequence of random floats on [0,1). Add sequences of 100 consecutive floats. The sums should be normally distributed with characteristic mean and sigma.
- **Runs Test**: Generate a long sequence of random floats on [0,1). Count ascending and descending runs. The counts should follow a certain distribution.
- **The Craps Test**: Play 200,000 games of craps, counting the wins and the number of throws per game and check the distribution.

RN with other distributions

- **Transformation method**

  Poisson distribution

  Gaussian distribution

  (Box Muller, 1958)

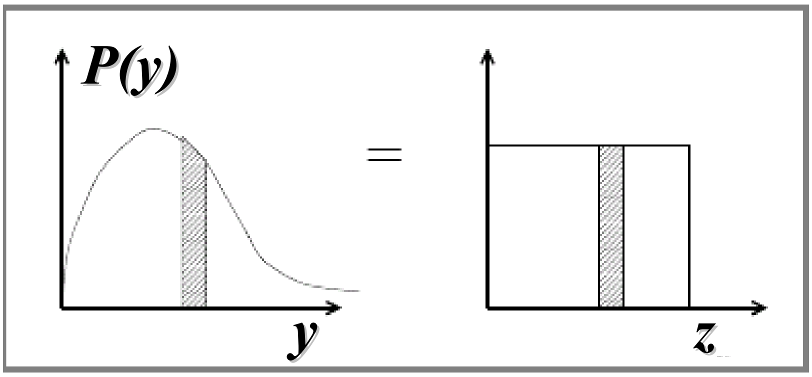
- **Rejection method**

Transformation method

We want random numbers *y* distributed as *P*(*y*).

Start with homogeneously distributed numbers *z*:

$$P(z) = \begin{cases} 1 & \text{if} \quad z \in [0,1] \\ 0 & \text{otherwise} \end{cases}$$



$$z = \int_0^z P(z')dz' = \int_0^y P(y')dy'$$

Transformation method

example:

generate Poisson distribution:

$$P(y) = ke^{-ky}$$

$$z = \int_0^y ke^{-ky'}dy' = [-e^{-ky}]_0^y = 1 - e^{-ky}$$

$$\Rightarrow \quad y = -\frac{1}{k}\ln(1-z)$$

where $z \in [0,1)$ are homogeneous random numbers.

This method only works if the integral can be solved and the resulting function can be inverted.

Box –Muller (1958)

Gaussian distribution:

$$P(y) = \frac{1}{\sqrt{\pi\sigma}} e^{-\frac{y^2}{\sigma}}$$

$$z = \int_0^y \frac{1}{\sqrt{\pi\sigma}} e^{-\frac{y^2}{\sigma}} dy$$

cannot be solved in closed form.

trick:

$$r^2 = y_1^2 + y_2^2$$

$$\tan\varphi = \frac{y_1}{y_2}$$

$$dy_1 dy_2 = r dr d\varphi$$

$$z_1 \cdot z_2 = \int_0^{y_1} \frac{1}{\sqrt{\pi\sigma}} e^{-\frac{y_1^2}{\sigma}} dy_1 \cdot \int_0^{y_2} \frac{1}{\sqrt{\pi\sigma}} e^{-\frac{y_2^2}{\sigma}} dy_2$$

$$= \frac{1}{\pi\sigma}\int_0^{y_1}\int_0^{y_2} e^{-\frac{y_1^2+y_2^2}{\sigma}} dy_1 dy_2 = \frac{1}{\pi\sigma}\int_0^{\varphi}\int_0^{r} e^{-\frac{r^2}{\sigma}} r dr d\varphi$$

$$= \frac{\varphi}{\pi\sigma}\frac{\sigma}{2}(1-e^{-\frac{r^2}{\sigma}}) = \frac{1}{2\pi}\arctan\left(\frac{y_1}{y_2}\right)(1-e^{-\frac{y_1^2+y_2^2}{\sigma}})$$

Box –Muller trick

$$z_1 \cdot z_2 = \frac{1}{2\pi}\arctan\left(\frac{y_1}{y_2}\right)\cdot\left(1-e^{-\frac{y_1^2+y_2^2}{\sigma}}\right)$$

$$y_1^2 + y_2^2 = -\sigma \ln\left(1-z_2\right)$$

$$\frac{y_1}{y_2} = \tan 2\pi z_1 = \frac{\sin 2\pi z_1}{\cos 2\pi z_1}$$

$$\Rightarrow$$

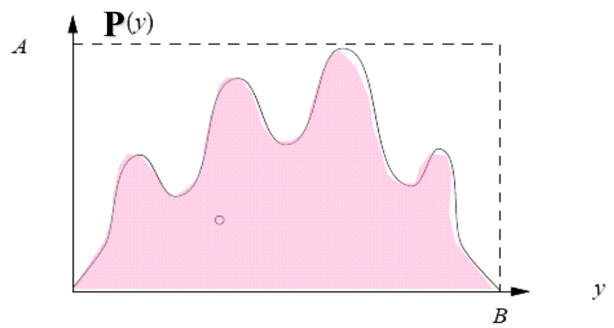
$$\boxed{\begin{aligned} y_1 &= \sqrt{-\sigma \ln\left(1-z_2\right)}\,\sin 2\pi z_1 \\ y_2 &= \sqrt{-\sigma \ln\left(1-z_2\right)}\,\cos 2\pi z_1 \end{aligned}}$$

From two homogeneously distributed random numbers z_1 and z_2 one gets two Gaussian distributed random numbers y_1 and y_2 .

Rejection method

Generate random numbers $y \in [0, B]$ sampled according to a distribution $P(y)$ with $P(y) < A$.

Sample two homogeneously distributed random numbers z_1 , $z_2 \in [0,1)$. If the point (Bz_1, Az_2) lies above the curve $P(y)$, i.e. $P(Bz_1) < Az_2$ then reject the attempt, otherwise $y = Bz_1$ is retained as a random number which is distributed according to $P(y)$.



Percolation

Broadbent and Hammersley
Proc. Cambridge Phil. Soc.
Vol. 53, p.629 (1957)

John M. Hammersley
(1920 – 2004)

References to percolation

- D. Stauffer: „Introduction to Percolation Theory“ (Taylor and Francis, 1985)
- D. Stauffer and A. Aharony: „Introduction to Percolation Theory, Revised Second Edition“ (Taylor and Francis, 1992)
- M. Sahimi: „Applications of Percolation Theory“ (Taylor and Francis, 1994)
- G. Grimmett: „Percolation“ (Springer, 1989)
- B.Bollobas and O.Riordan: „Percolation“ (Cambridge Univ. Press, 2006)

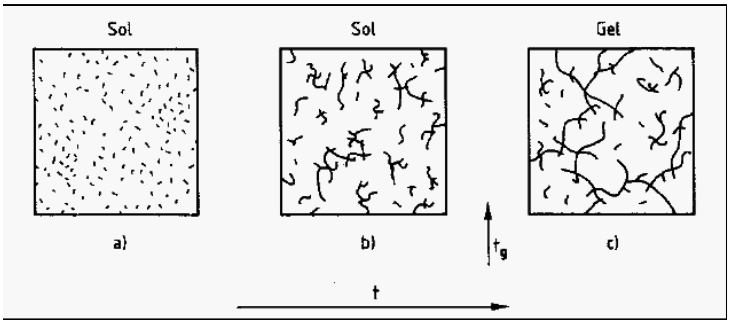
Percolator

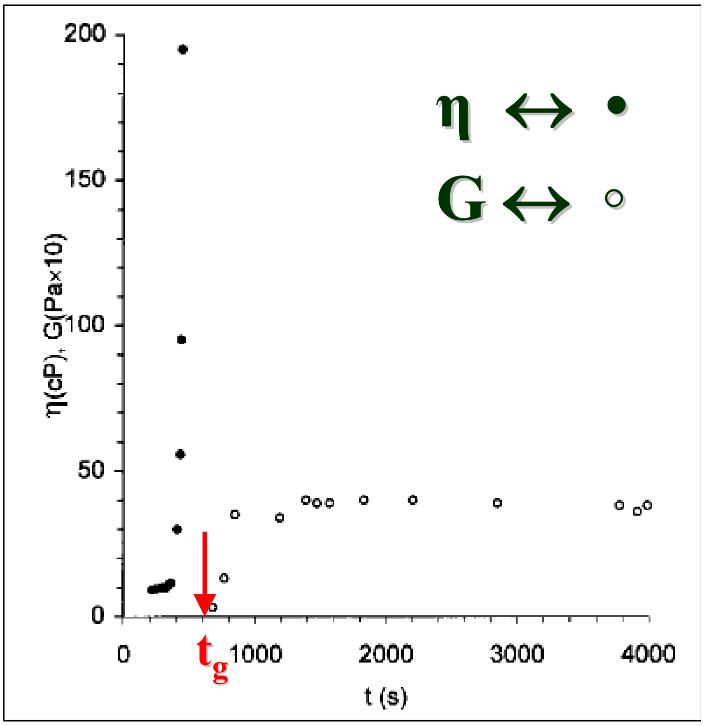
Applications of percolation

- Porous media (oil production, pollution of soils)
- Sol-gel transition
- Mixtures of conductors and insulators
- Forest fires
- Propagation of epidemics or computer virus
- Crash of stock markets (Sornette)
- Landslide election victories (Galam)
- Recognition of antigens by T-cells (Perelson)
- …

Gelatin formation

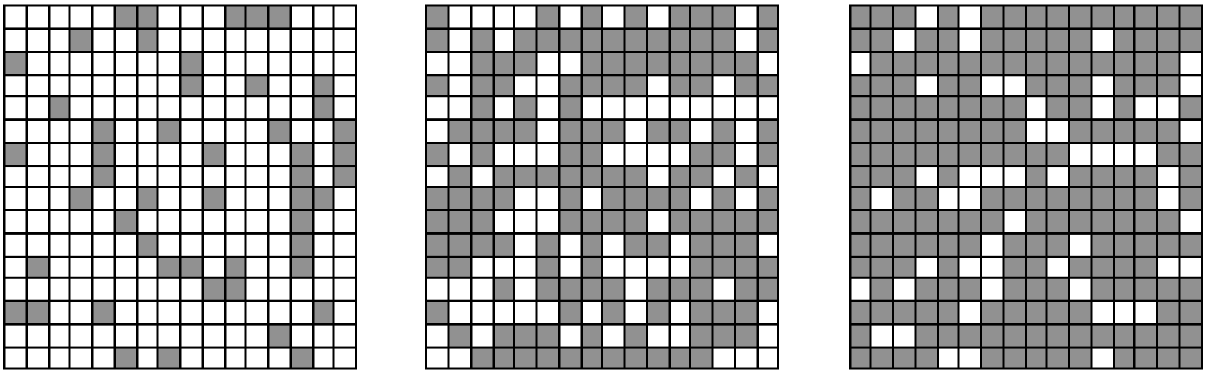
Sol -gel transition





Shear modulus G vanishes and viscosity η diverges at t_g as function of time t.

Percolation



p = 0.2 p = 0.59 p = 0.8

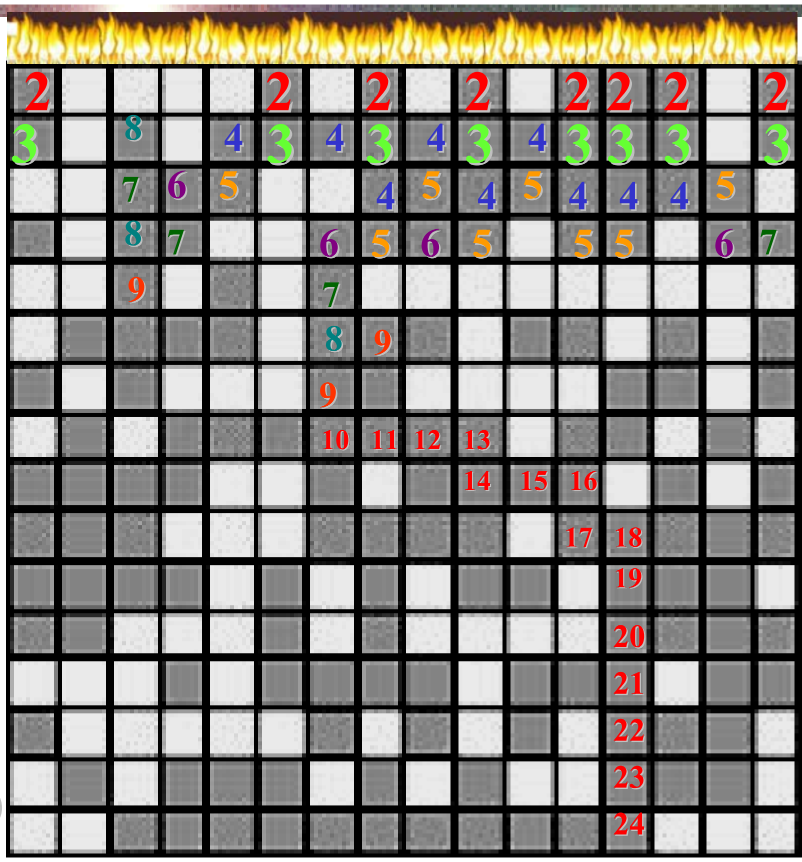
site percolation on square lattice

p is the probability to occupy a site.

bla

Neighboring occupied sites are „connected“ and belong to the same cluster.

Burning method



$p = 0.59$

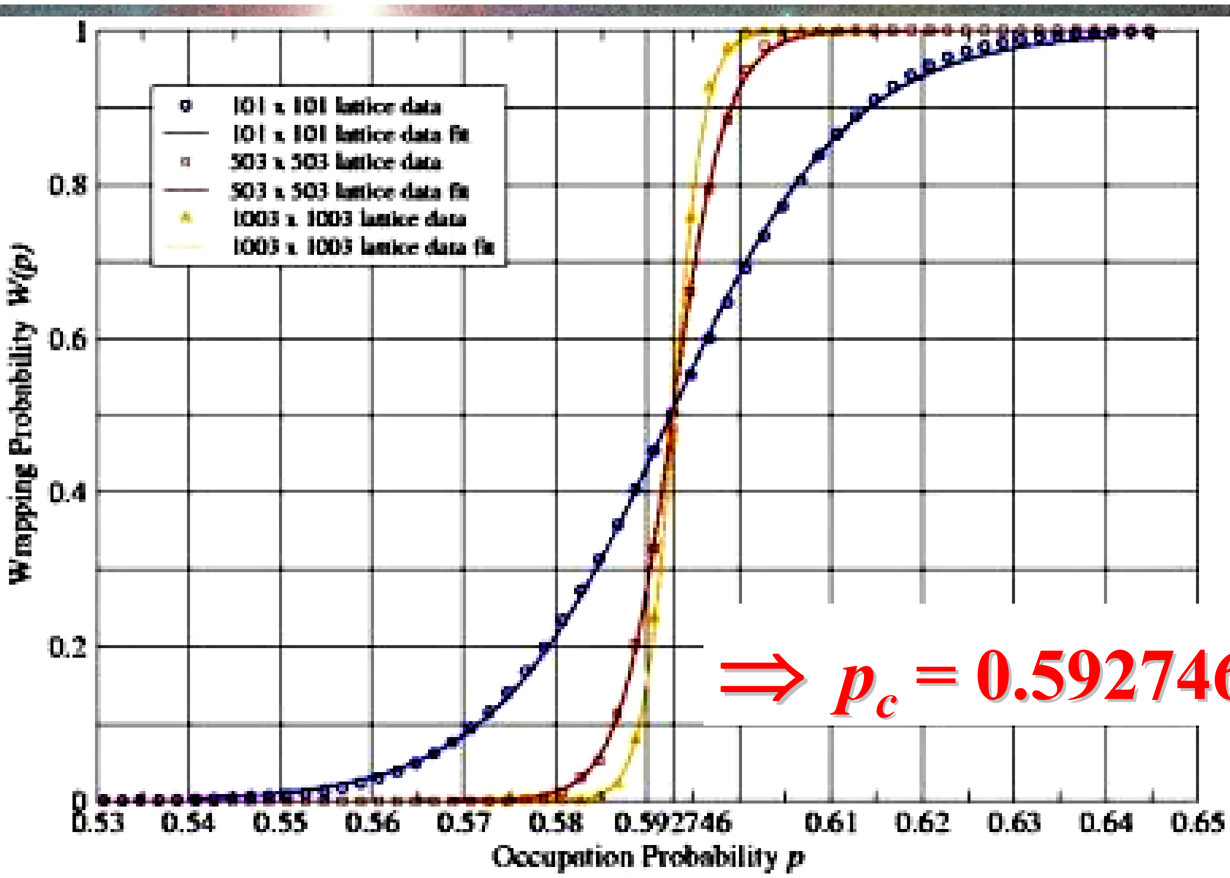
$L = 16$

shortest path

$t_s = 24$

HH et al (1984)

Probability to find a spanning cluster



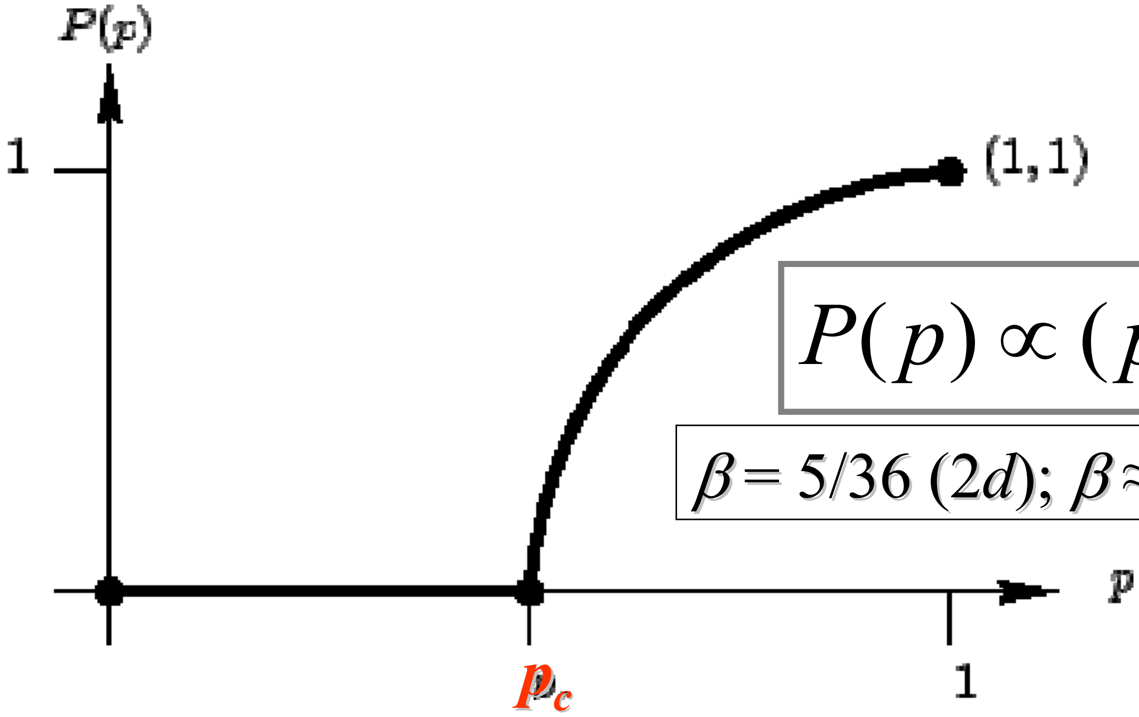
$\Rightarrow p_c = 0.592746...$

Percolation thresholds p_c

lattice	site	bond
cubic (body-centered)	0.246	0.1803
cubic (face-centered)	0.198	0.119
cubic (simple)	0.3116	0.2488
diamond	0.43	0.388
honeycomb	0.6962	0.65271*
4-hypercubic	0.197	0.1601
5-hypercubic	0.141	0.1182
6-hypercubic	0.107	0.0942
7-hypercubic	0.089	0.0787
square	0.592746	0.50000*
triangular	0.50000*	0.34729*

Order parameter of percolation

***P*(*p*) = fraction of sites in the largest cluster**



$$P(p) \propto (p_c - p)^{\beta}$$

$\beta = 5/36$ (2d); $\beta \approx 0.41$ (3d)

Many clusters

bond percolation

We have clusters of different sizes s and can study the cluster size distribution n_s

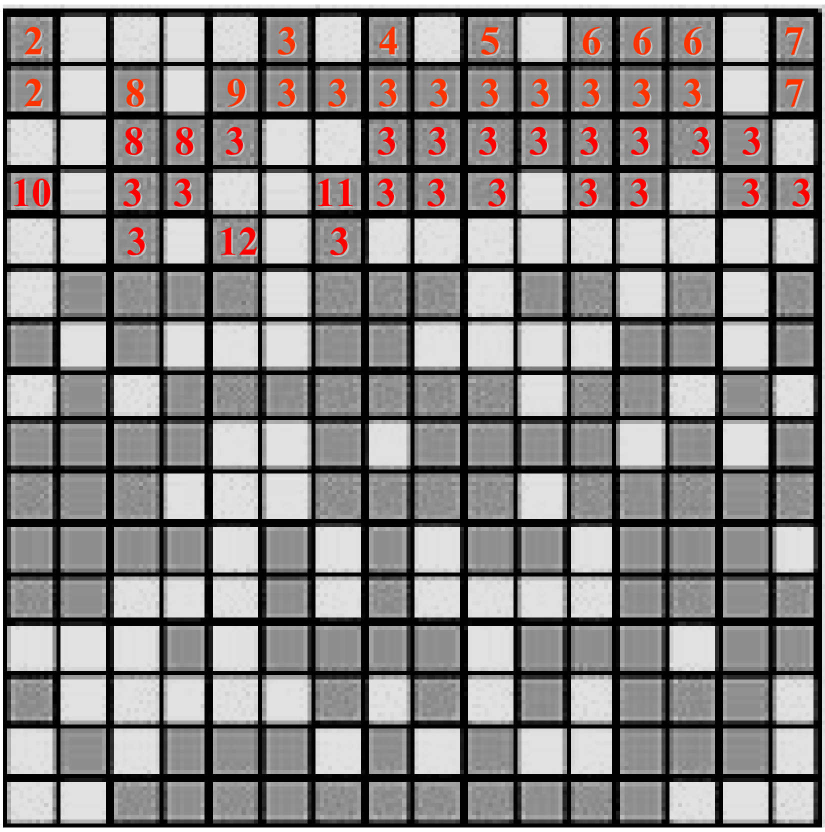
$$\boxed{n_s = \frac{N_s}{N}}$$

Cluster size distribution

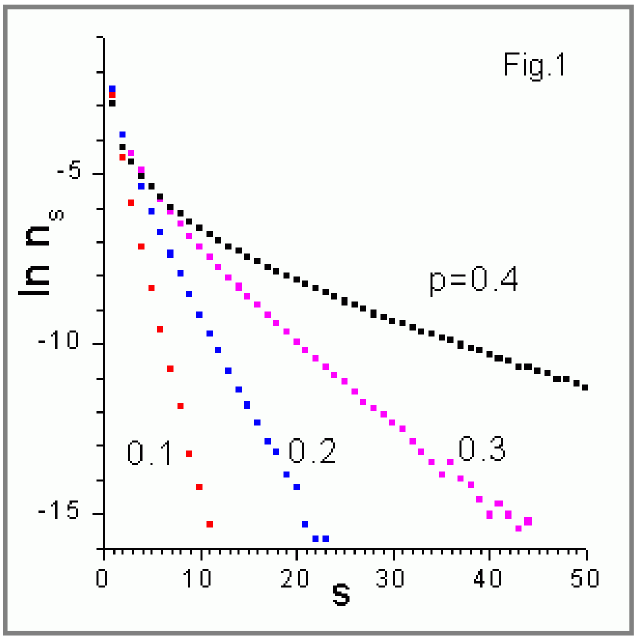
Hoshen-Kopelman Algorithm (1976)

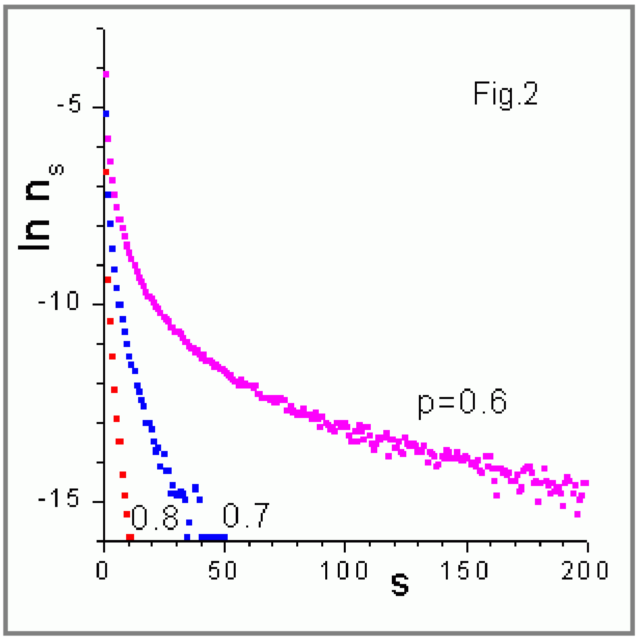
- $N(i,j) \in \{0,1\}$, 0 = empty, 1 = occupied
- Start: $k = 2$, N(first occupied site) = k, $M(k) = 1$
- If site top and left are empty: $k = k + 1$ and continue
- If one of them has value k_0: $N(i,j) = k_0$, $M(k_0) = M(k_0) + 1$
- If both are occupied with k_1 and k_2: choose one, e.g. k_1, $N(i,j) = k_1$, $M(k_1) = M(k_1) + M(k_2) + 1$, $M(k_2) = -k_1$
- If any k has negative M(k): `while(M(k)<0)k=-M(k)`
- At end: `for(k=2; k<=kmax; k++) n(M(k))=n(M(k))+1`

Evolution of N(i,j)



Cluster size distribution n_s

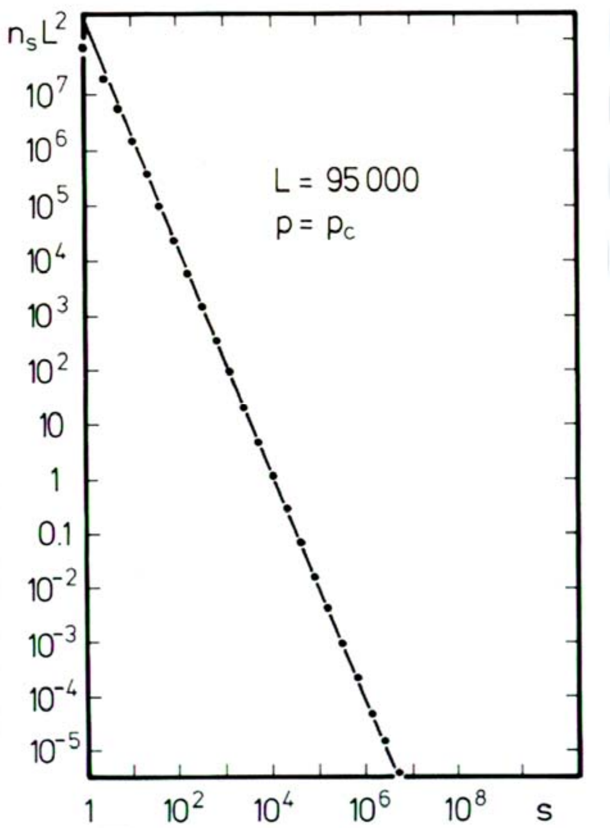




$$n_s(p < p_c) \propto s^{-\theta} e^{-as}$$

$$n_s(p > p_c) \propto e^{-bs^{(1-1/d)}}$$

Cluster size distribution at p_c



at p_c

$$n_s \propto s^{-\tau}$$

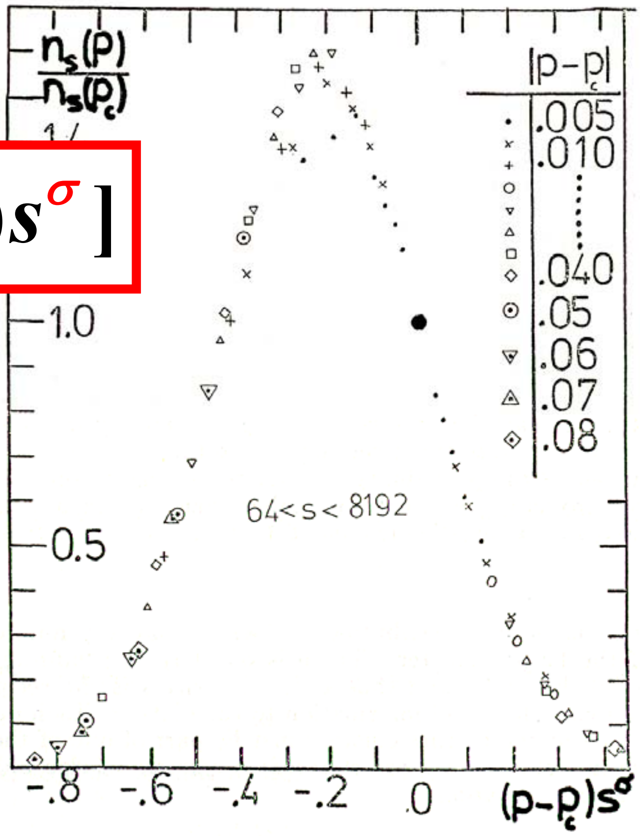
$$\tau = \begin{cases} \frac{187}{91} & \text{in} \quad 2d \\ 2.18 & \text{in} \quad 3d \end{cases}$$

$$2 \le \tau \le \frac{5}{2}$$

Scaling of cluster size distribution

s = size of cluster

$$\boxed{n_s(p) = s^{-\tau}\Re_{\pm}[(p-p_c)s^{\sigma}]}$$



Second moment χ

$$\boxed{\chi = < \sum_s' s^2 n_s >}$$

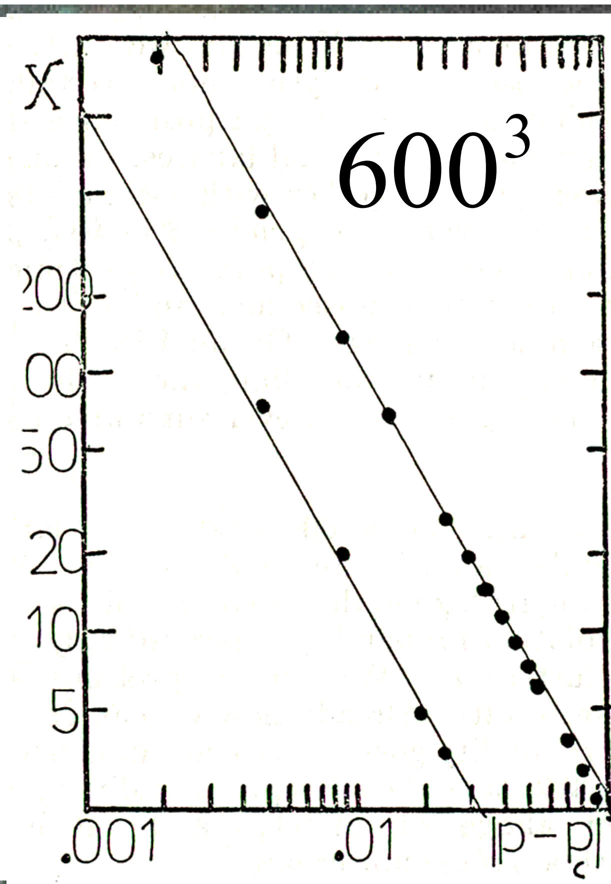
' means that one excludes the largest cluster

$$\boxed{\chi \propto C_{\pm}|p-p_c|^{-\gamma}}$$

$\gamma = 43/18 \approx 2.39$ (2*d*)

$\gamma \approx 1.80$ (3*d*)

$$\boxed{\gamma = \frac{3-\tau}{\sigma}}$$



Critical exponents

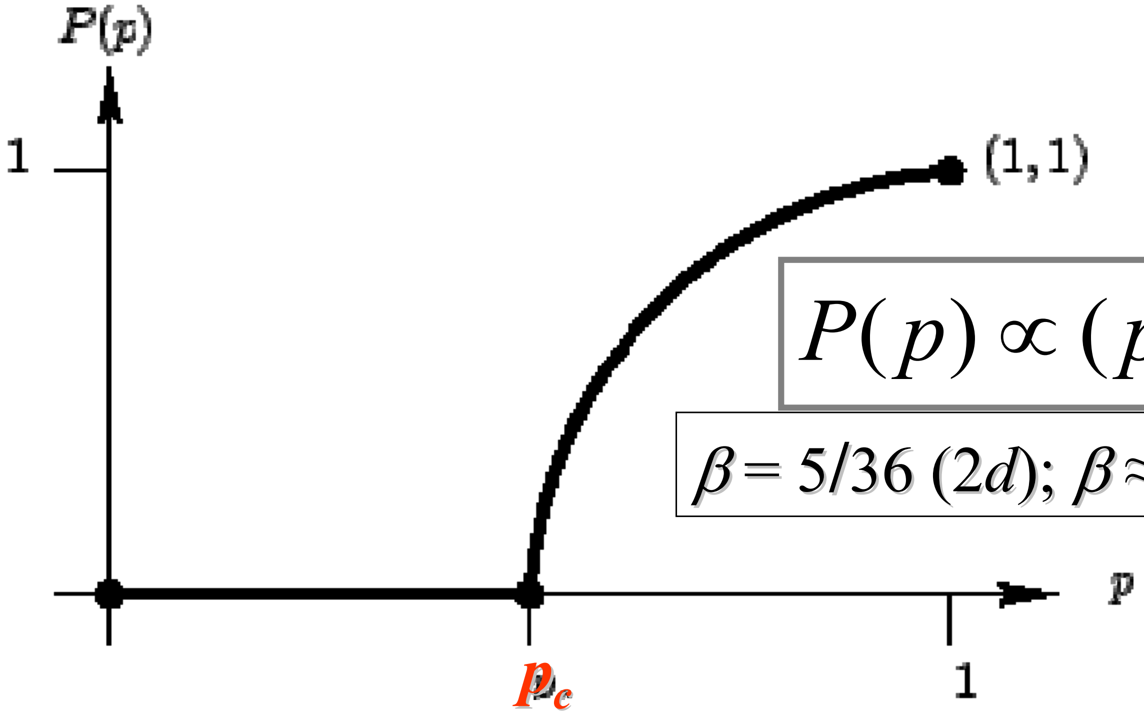
Table 2. Percolation exponents for $d = 2, 3, 4, 5, 6-\varepsilon$ and in the Bethe lattice together with the page number defining the exponent. Rational numbers give (presumably) exact results, whereas those with a decimal fraction are numerical estimates.

Exponent	$d=2$	$d=3$	$d=4$	$d=5$	$d=6-\varepsilon$	Bethe	Page
α	$-2/3$	$-0{\cdot}62$	$-0{\cdot}72$	$-0{\cdot}86$	$-1+\varepsilon/7$	-1	39
β	$5/36$	$0{\cdot}41$	$0{\cdot}64$	$0{\cdot}84$	$1-\varepsilon/7$	1	37
γ	$43/18$	$1{\cdot}80$	$1{\cdot}44$	$1{\cdot}18$	$1+\varepsilon/7$	1	37
ν	$4/3$	$0{\cdot}88$	$0{\cdot}68$	$0{\cdot}57$	$\frac{1}{2}+5\varepsilon/84$	$1/2$	60
σ	$36/91$	$0{\cdot}45$	$0{\cdot}48$	$0{\cdot}49$	$\frac{1}{2}+O(\varepsilon^2)$	$1/2$	35
τ	$187/91$	$2{\cdot}18$	$2{\cdot}31$	$2{\cdot}41$	$\frac{5}{2}-3\varepsilon/14$	$5/2$	33
$D(p=p_c)$	$91/48$	$2{\cdot}53$	$3{\cdot}06$	$3{\cdot}54$	$4-10\varepsilon/21$	4	10
$D(p<p_c)$	$1{\cdot}56$	2	$12/5$	$2{\cdot}8$	–	4	62
$D(p>p_c)$	2	3	4	5	–	4	62
$\zeta(p<p_c)$	1	1	1	1	–	1	56
$\zeta(p>p_c)$	$1/2$	$2/3$	$3/4$	$4/5$	–	1	56
$\theta(p<p_c)$	1	$3/2$	$1{\cdot}9$	$2{\cdot}2$	–	$5/2$	54
$\theta(p>p_c)$	$5/4$	$-1/9$	$1/8$	$-449/450$	–	$5/2$	54
$f_{\max}$	$5{\cdot}0$	$1{\cdot}6$	$1{\cdot}4$	$1{\cdot}1$		1	42
μ	$1{\cdot}30$	$2{\cdot}0$	$2{\cdot}4$	$2{\cdot}7$	$3-5\varepsilon/21$	3	91
s	$1{\cdot}30$	$0{\cdot}73$	$0{\cdot}4$	$0{\cdot}1_5$		0	93
D_B	$1{\cdot}6$	$1{\cdot}7_4$	$1{\cdot}9$	$2{\cdot}0$	$2+\varepsilon/21$	2	95
$D_{\min}(p=p_c)$	$1{\cdot}13$	$1{\cdot}34$	$1{\cdot}5$	$1{\cdot}8$	$2-\varepsilon/6$	2	97
$D_{\min}(p<p_c)$	$1{\cdot}17$	$1{\cdot}36$	$1{\cdot}5$		–	2	98
$D_{\max}(p=p_c)$	$1{\cdot}4$	$1{\cdot}6$	$1{\cdot}7$	$1{\cdot}9$	$2-\varepsilon/42$	2	97

For the exponents at p_c, the Bethe lattice values are exact at $d \geqslant 6$. A dash means that 6 is not the upper critical dimension for the ε-expansion.

Order parameter of percolation

***P*(*p*) = fraction of sites in the largest cluster**



$$P(p) \propto (p_c - p)^{\beta}$$

$\beta = 5/36\ (2d)$; $\beta \approx 0.41\ (3d)$

Size dependence of OP

L is linear size of the system

at p_c:

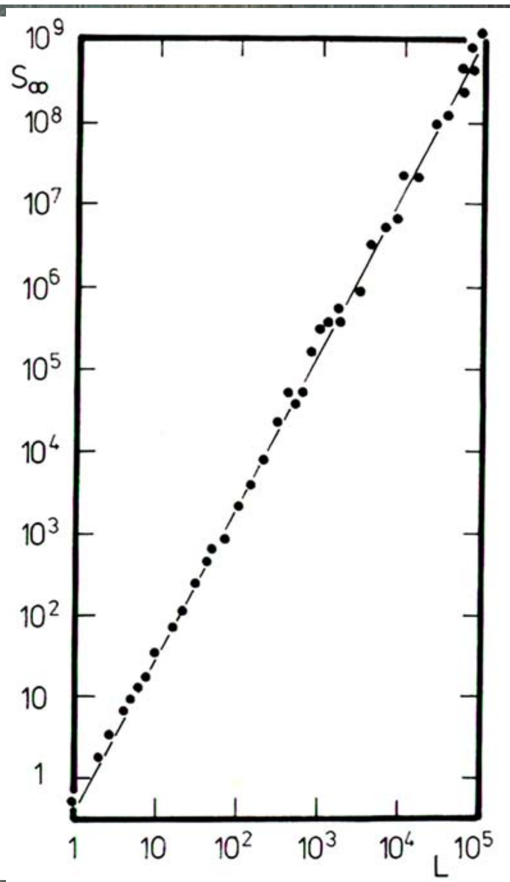
$$PL^d = s_\infty \propto L^{d_f}$$

$d_f = 91/48$ in $d = 2$

$d_f \approx 2.51$ in $d = 3$

We will show later:

$$d_f = d - \frac{\beta}{\nu}$$



Shortest path t_s at p_c

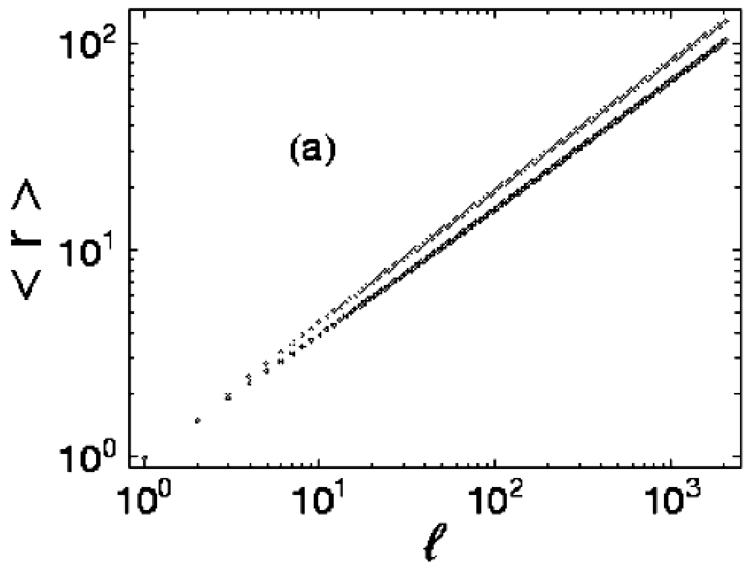
also called „chemical distance“ ℓ

$$t_s \propto L^{d_{\min}}$$

$d_{min} \approx 1.13$ (2d)

$d_{min} \approx 1.33$ (3d)

$d_{min} \approx 1.61$ (4d)



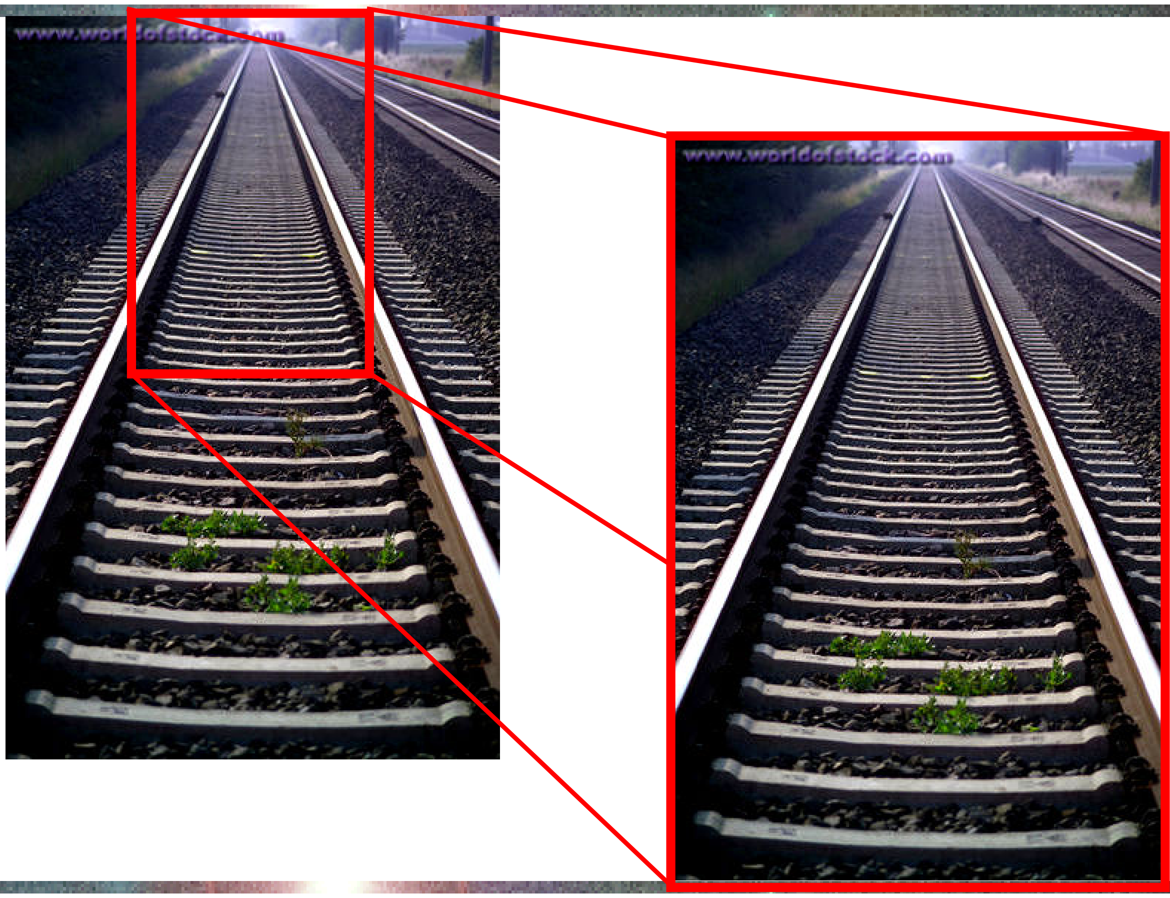
site (upper) and bond (lower) percolation in 4 dimensions (Ziff, 2001)

Fractal dimension

Books:

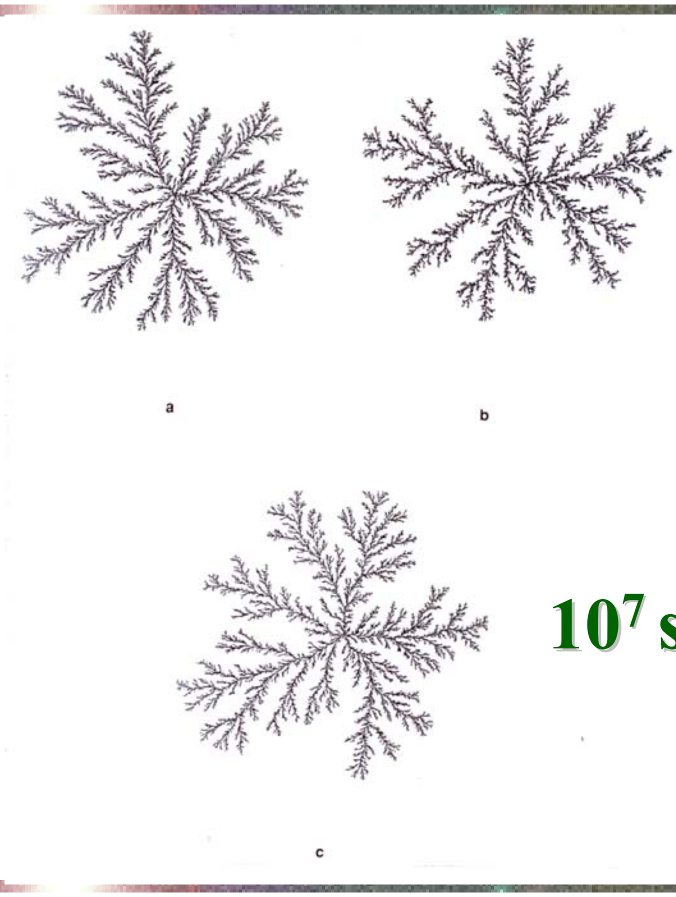
- B.B.Mandelbrot, „Les Objets Fractals: Forme Hazard et Dimension“ (Flammarion, Paris,1975)
- J. Feder, „Fractals“ (Plenum Press, NY, 1988)
- T. Vicsek, „Fractal Growth Phenomena“ (World Scientific, Singapore, 1989)
- H.-O.Peitgen and P.H.Richter, „The Beauty of Fractals“ (Springer, Berlin, 1986)
- J.-F. Gouyet, „Physique et Structures Fractales) (Masson, Paris, 1992)

Self similarity



Self similarity

10^5 sites



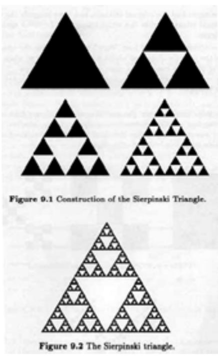
10^6 sites

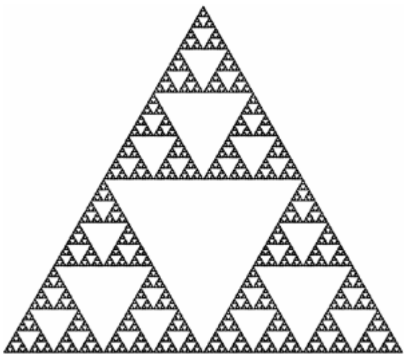
10^7 sites

DLA clusters

Fractal dimension

Sierpinski gasket



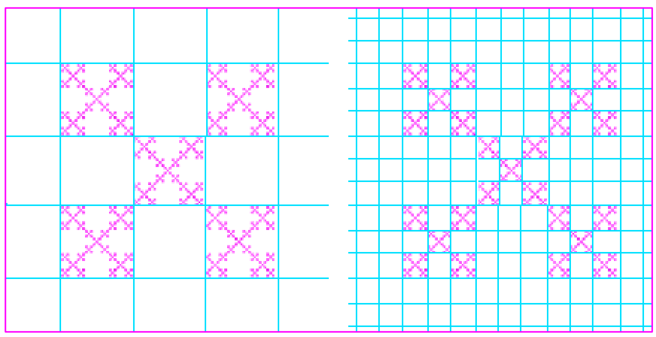


$$\boxed{M \propto L^{d_f}}$$

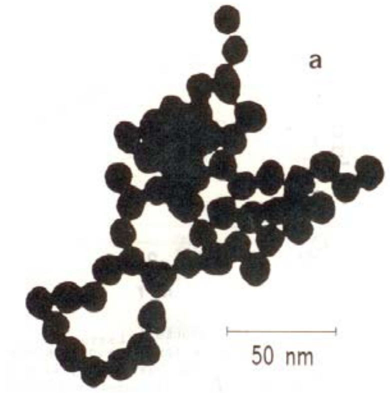
$d_f = \log(3)/\log(2) \approx 1.602$

„box counting“ method:

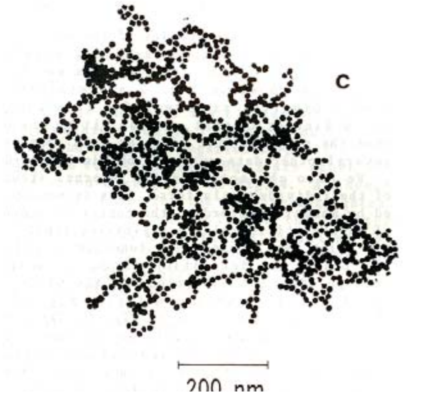
$d_f = \log(5)/\log(3) \approx 1.46$

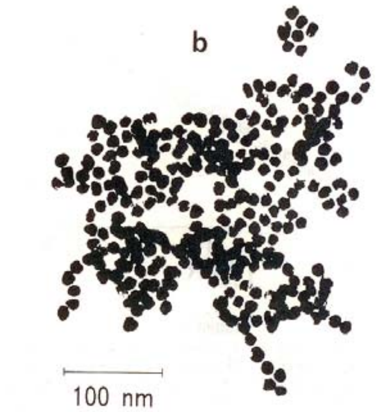


Gold colloids

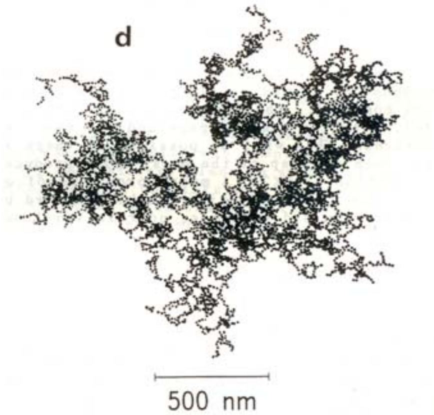


$d_f = 1.70$



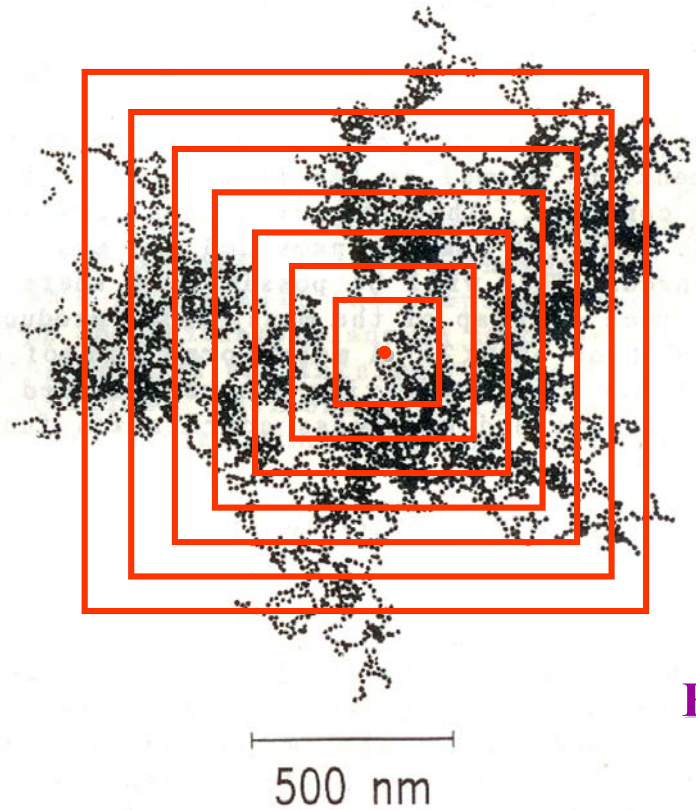


David Weitz, 1984



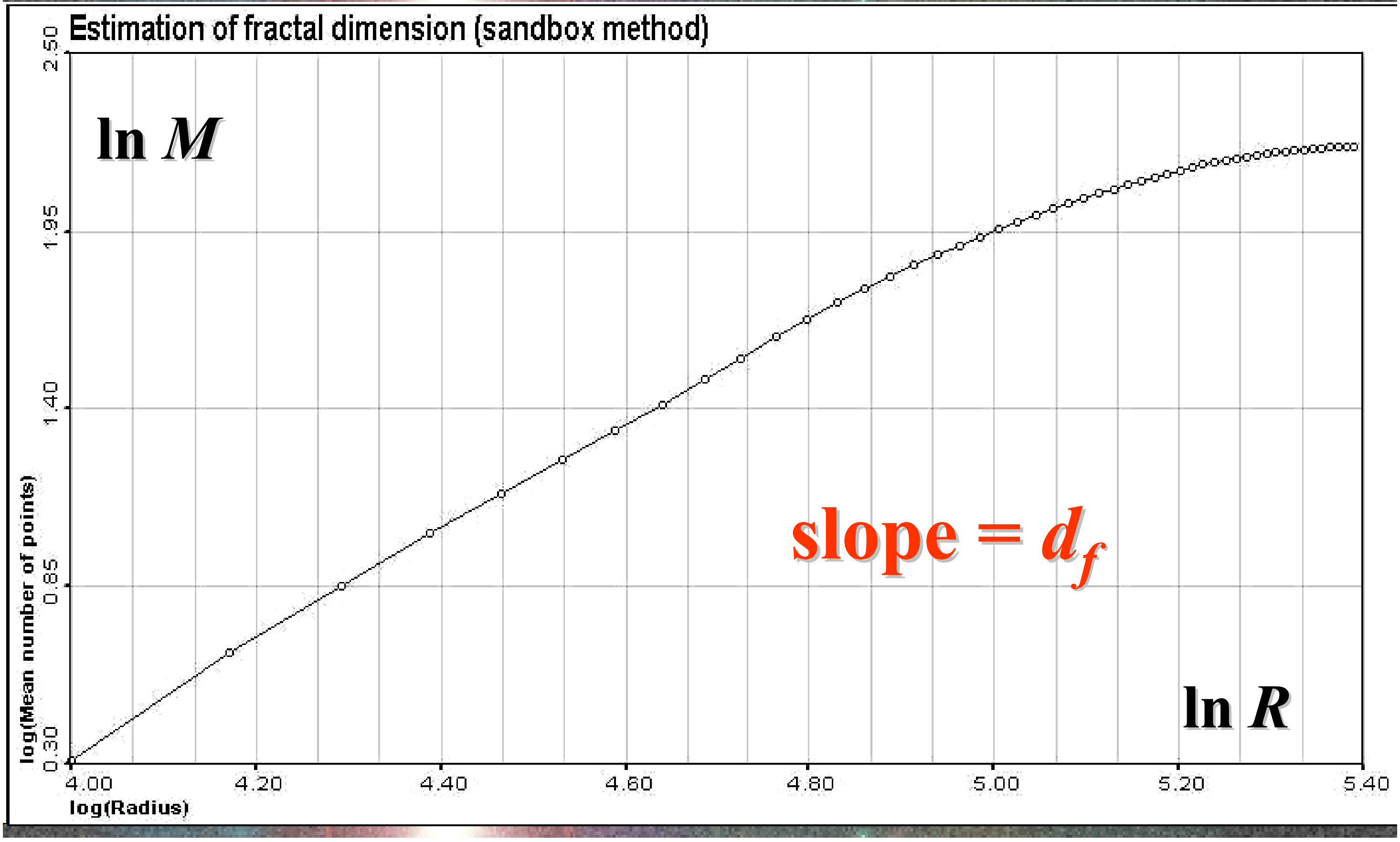
Sand-box method

$M(R)$ is the number of particles in box of size R



Forrest and Witten (1979)

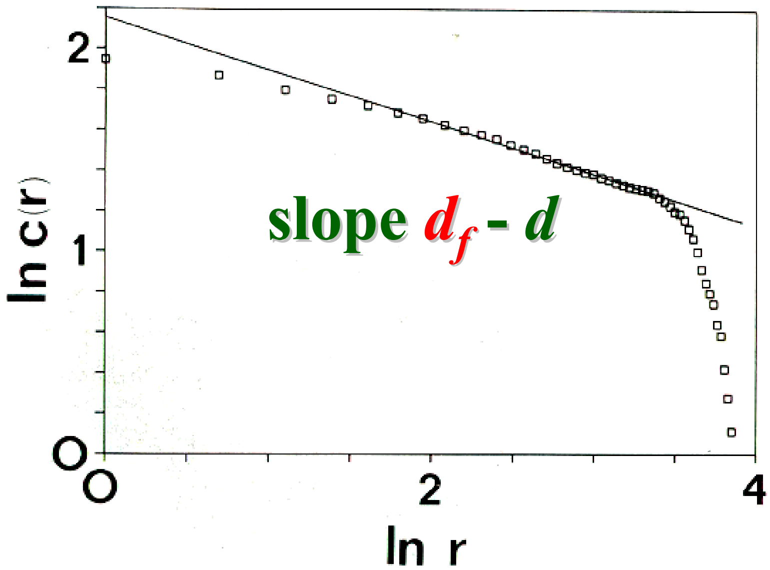
Sand-box method



Correlation function method

$$c(r) = \langle \rho(0)\rho(r) \rangle$$

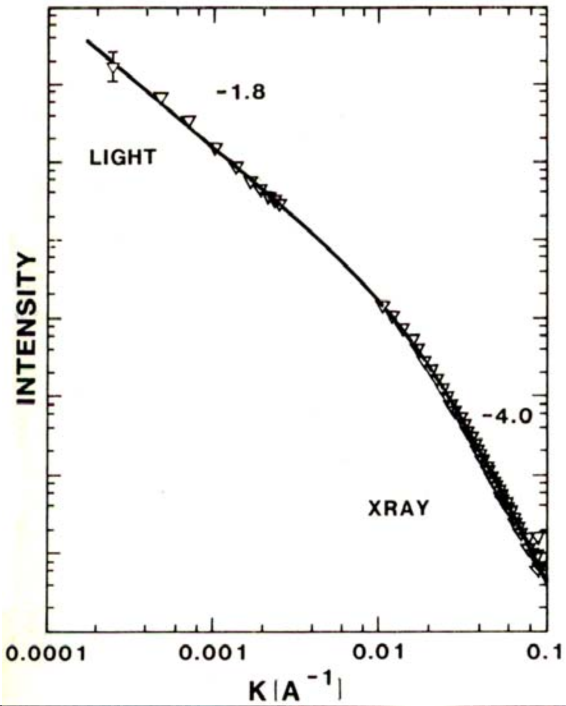
$$c(r) \propto r^{d_f - d}$$



$$c(r) = \frac{\Gamma(d/2)}{2\pi^{d/2} r^{d-1} \Delta r}\left[M(r+\Delta r) - M(r)\right]$$

Light scattering

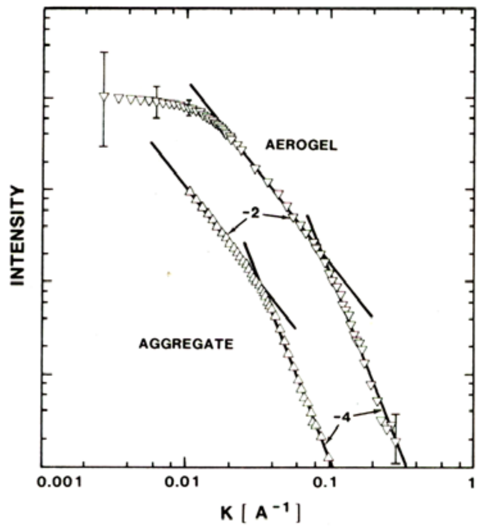
Intensity of scattered light with wavevector q:



$$I(q) \propto \int_{-\infty}^{\infty} c(r) e^{-qr} d^d r \propto q^{-d_f}$$

silica gel

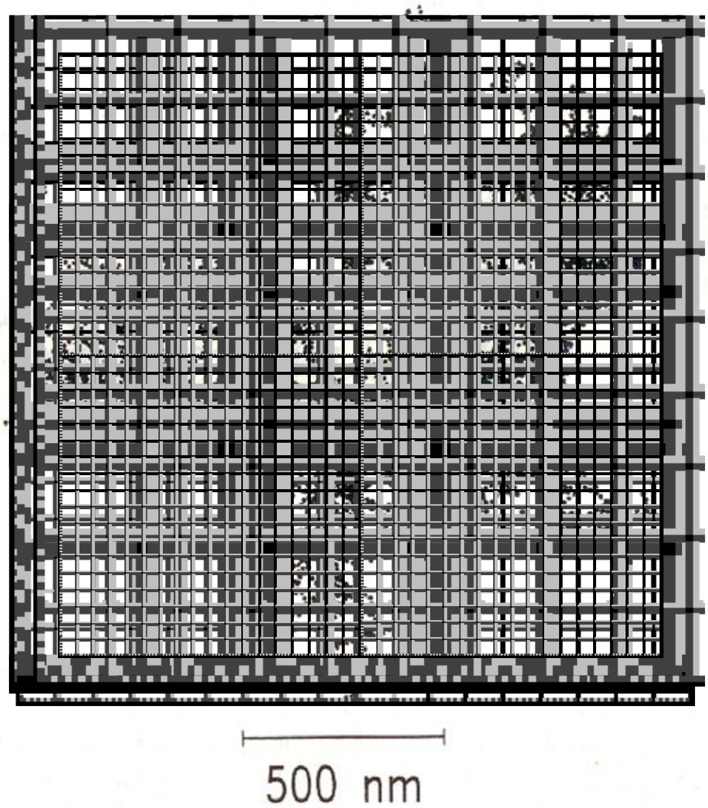
Schaefer (1984)



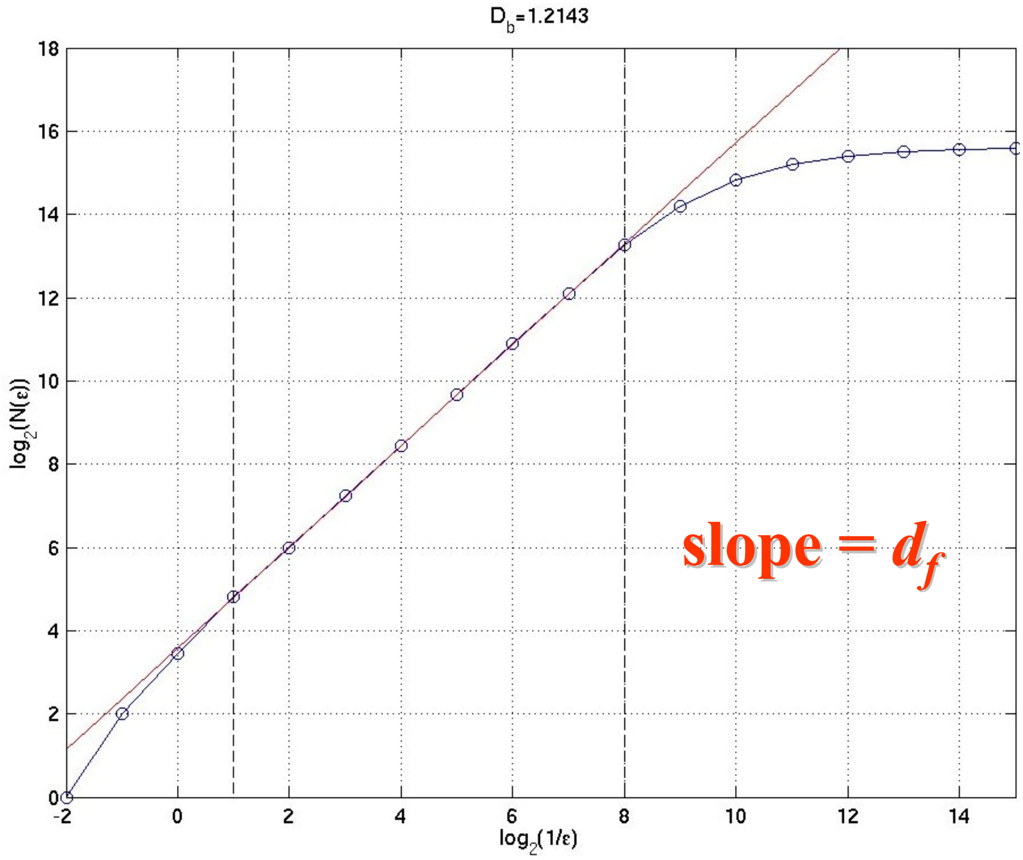
Box-counting method

ε = grid spacing

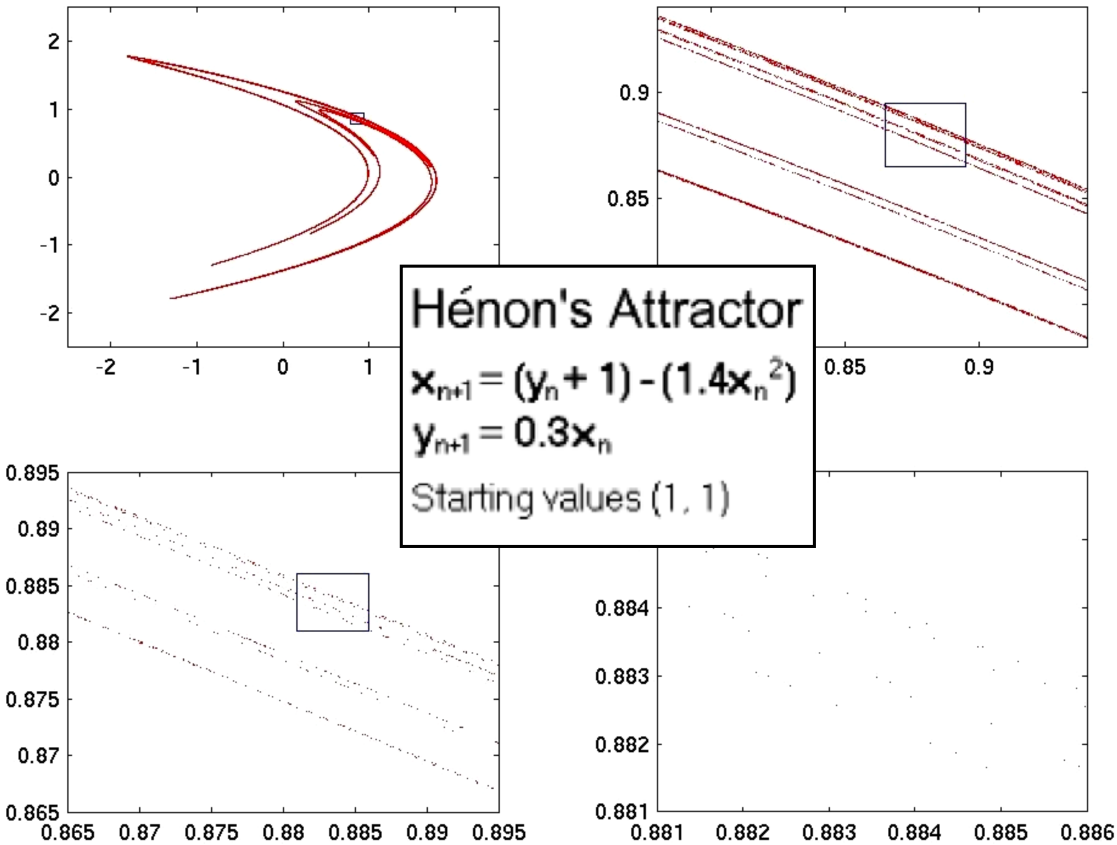
N(ε) = number of occupied cells



Box-counting method



Strange attractor



Multifractality

N_i = number of points in box i

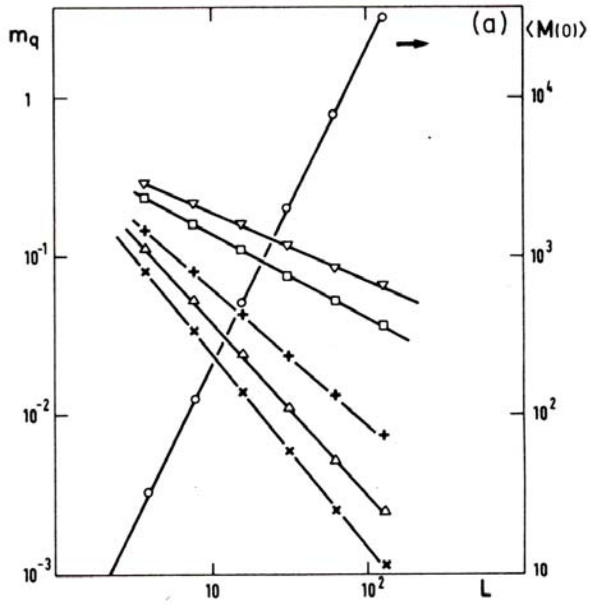
$p_i = N_i$ / total number of points

$$M_q = \sum_i p_i^q$$

$$M_q \propto L^{d_q}$$

$$m_q = (M_q / M_0)^{1/q}$$

$$d_q = \frac{1}{q-1} \lim_{\varepsilon \to 0} \lim_{N \to \infty} \frac{\ln m_q}{\ln \varepsilon}$$



Many clusters

bond percolation

Ensemble method

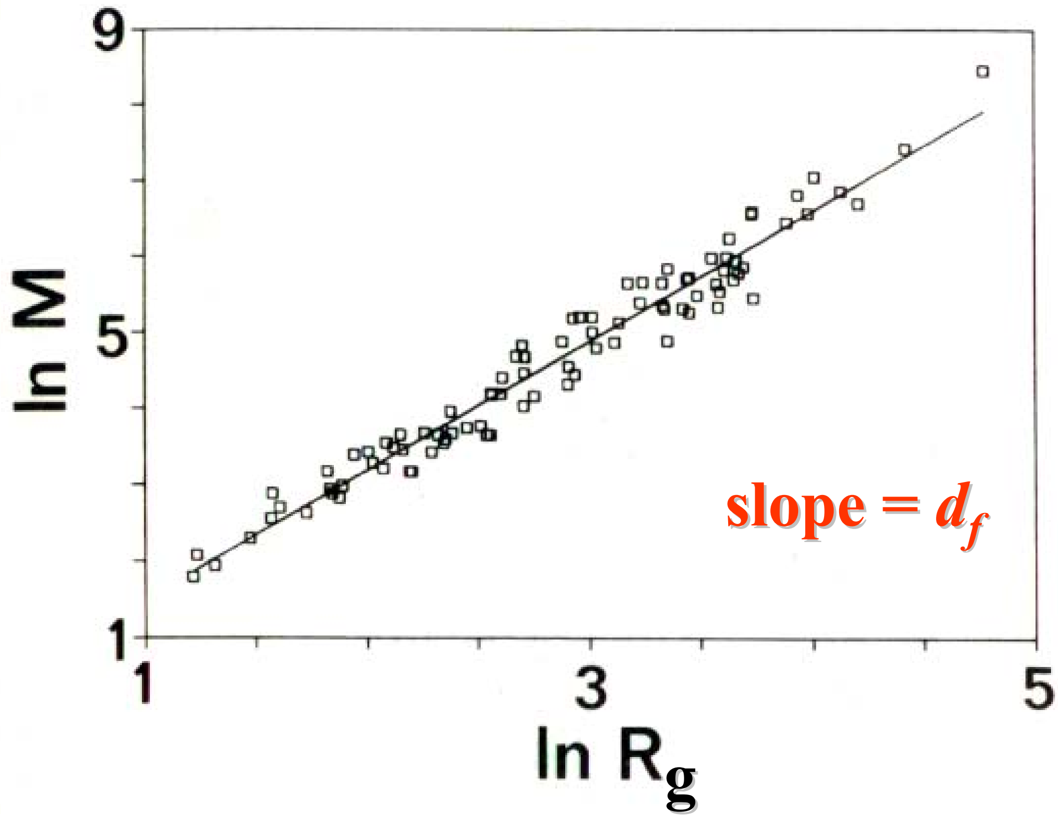
Take cluster of M sites.

Define „radius of gyration“ R_g:

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

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

Ensemble method



Percolation

The correlation function $g(r)$ for percolation describes the connectivity and is defined as the probability that an occupied site is connected to a site at distance r. This is equivalent to the probability that the two sites belong to the same cluster.

The correlation length ξ is the characteristic length of the exponential decay of the correlation function.

Correlation length ξ

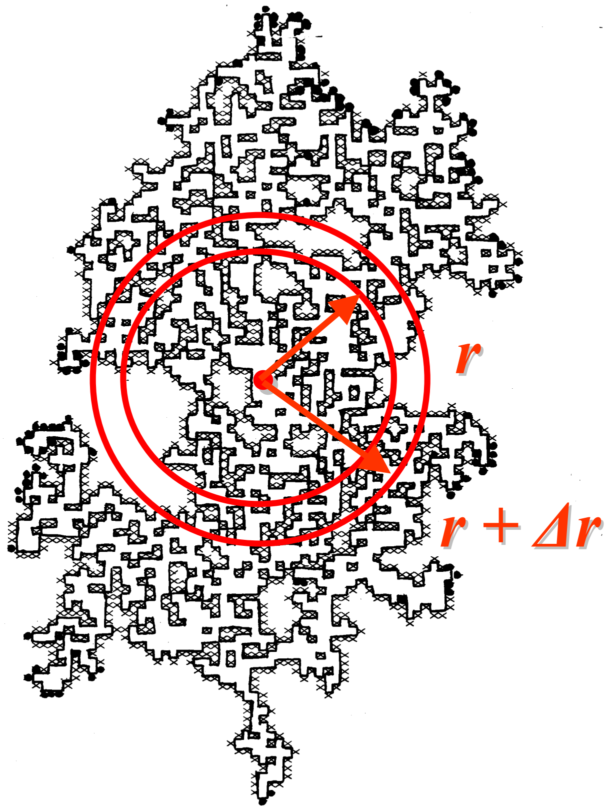
If one just analyses one cluster connectivity correlation function $g(r) = c(r)$

$$\boxed{g(r) = \frac{\Gamma(d/2)}{2\pi^{d/2} r^{d-1} \Delta r}[M(r+\Delta r) - M(r)]}$$

$$\boxed{g(r) \propto C + e^{-\frac{r}{\xi}} \quad \text{with} \quad C = 0 \quad \text{for} \quad p < p_c}$$

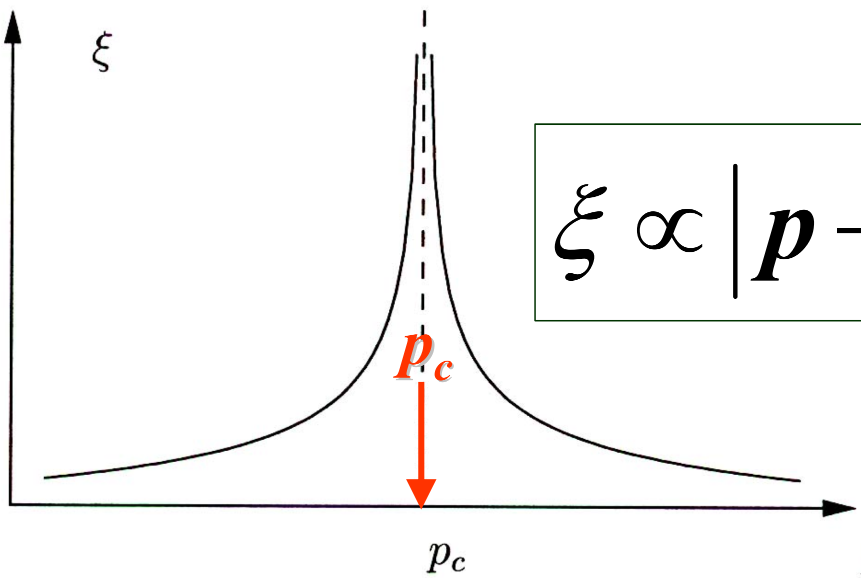
For $p < p_c$ the correlation length ξ is proportional to the radius of a typical cluster.

Calculate $g(r)$



Correlation length ξ

$$\nu = \begin{cases} 4/3 & \text{in 2 Dimensionen} \\ 0.88 & \text{in 3 Dimensionen} \end{cases}$$

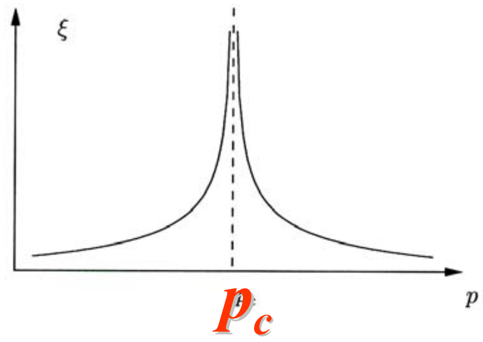


$$\xi \propto \left| p - p_c \right|^{-\nu}$$

Correlation length ξ

$$\boxed{\xi \propto |p - p_c|^{-\nu}}$$

$$\nu = \begin{cases} 4/3 & \text{in 2 Dimensionen} \\ 0.88 & \text{in 3 Dimensionen} \end{cases}$$



at p_c:

$$\boxed{g(r) \propto r^{-(d-2+\eta)}}$$

$\eta =$	5/24	2d
$\eta \approx$	-0.05	3d

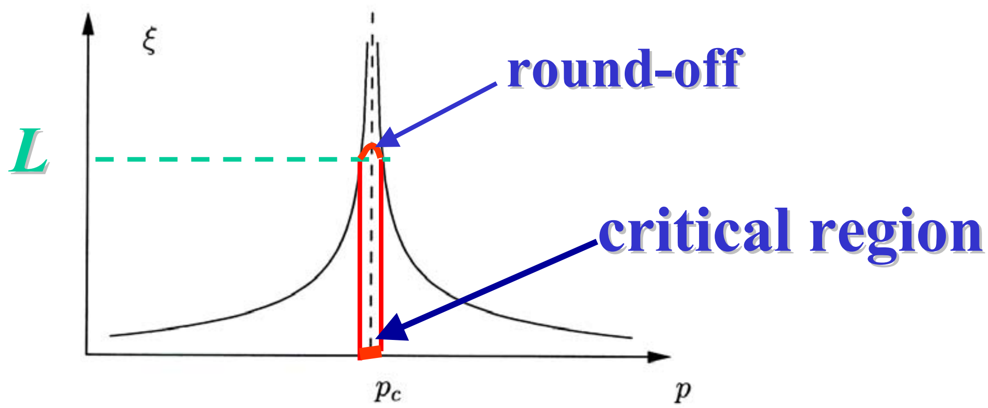
Finite size effects

problem when:

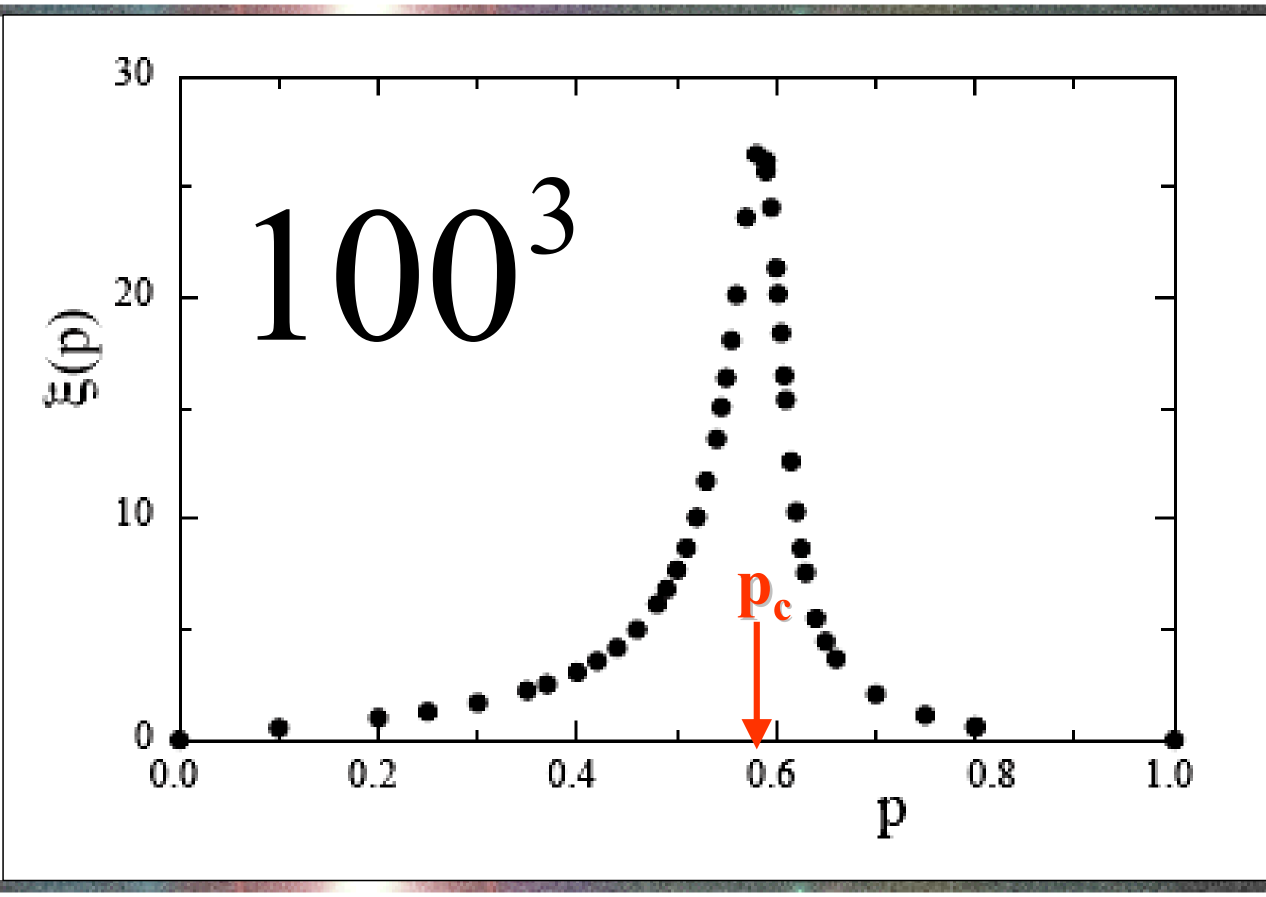
system size L < correlation length ξ

i.e. close to the critical point:

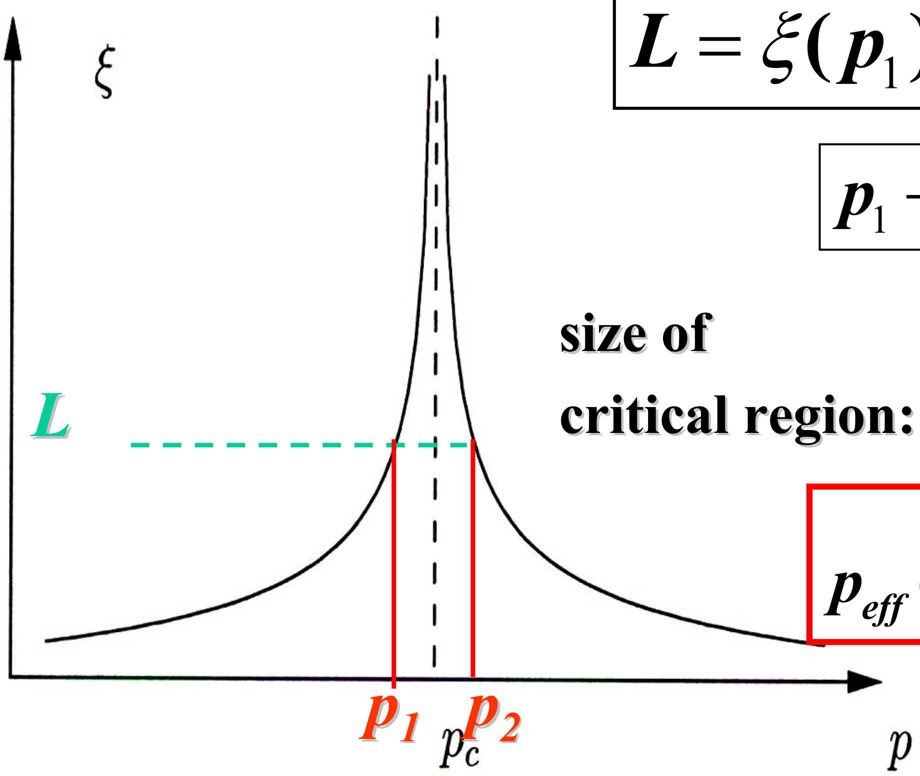
$$\nu = \begin{cases} 4/3 & \text{in 2 Dimensionen} \\ 0.88 & \text{in 3 Dimensionen} \end{cases}$$



Round-off in correlation length ξ



Finite size effects



$$L = \xi(p_1) \propto (p_1 - p_c)^{-\nu}$$

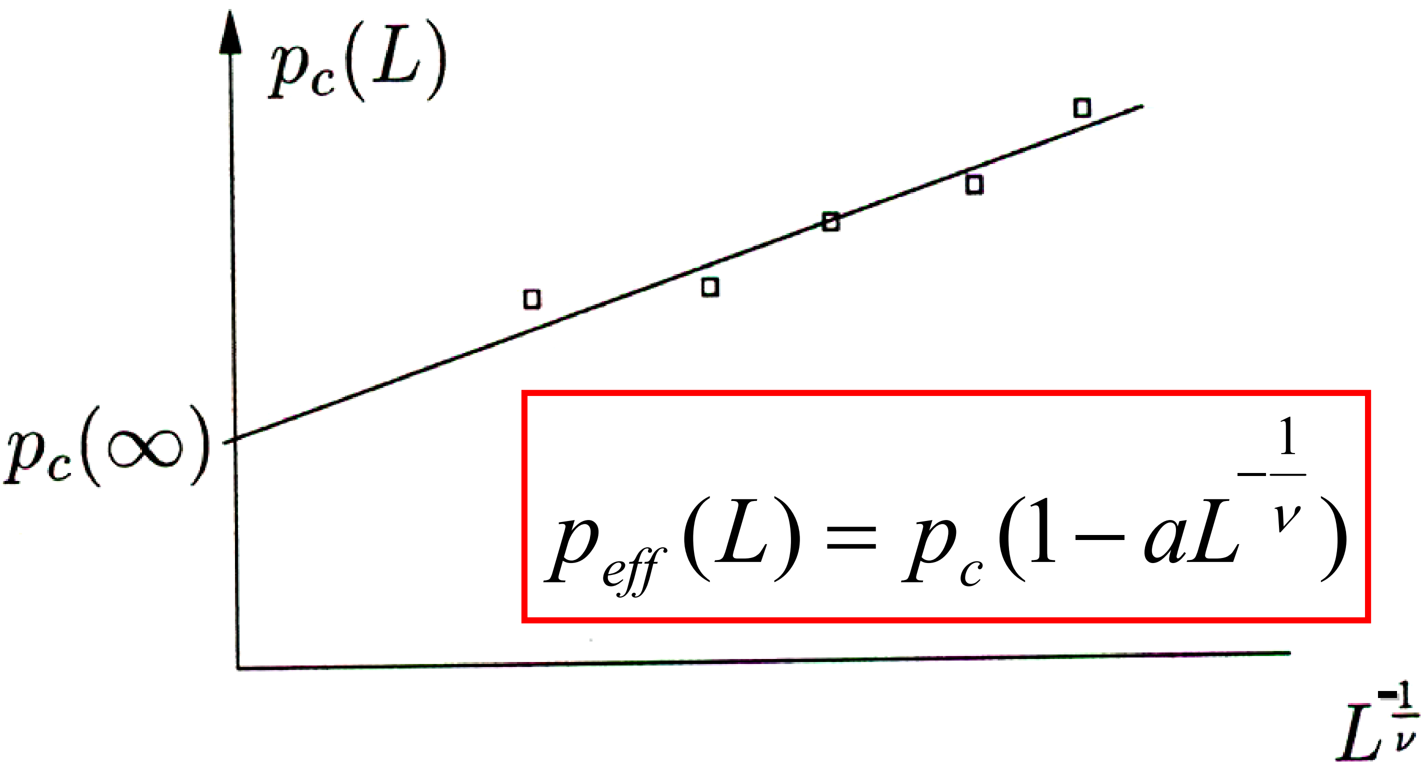
$$p_1 - p_2 = 2(p_1 - p_c)$$

size of critical region: $p_1 - p_2 \propto L^{-\frac{1}{\nu}}$

$$p_{eff}(L) = p_c(1 - aL^{-\frac{1}{\nu}})$$

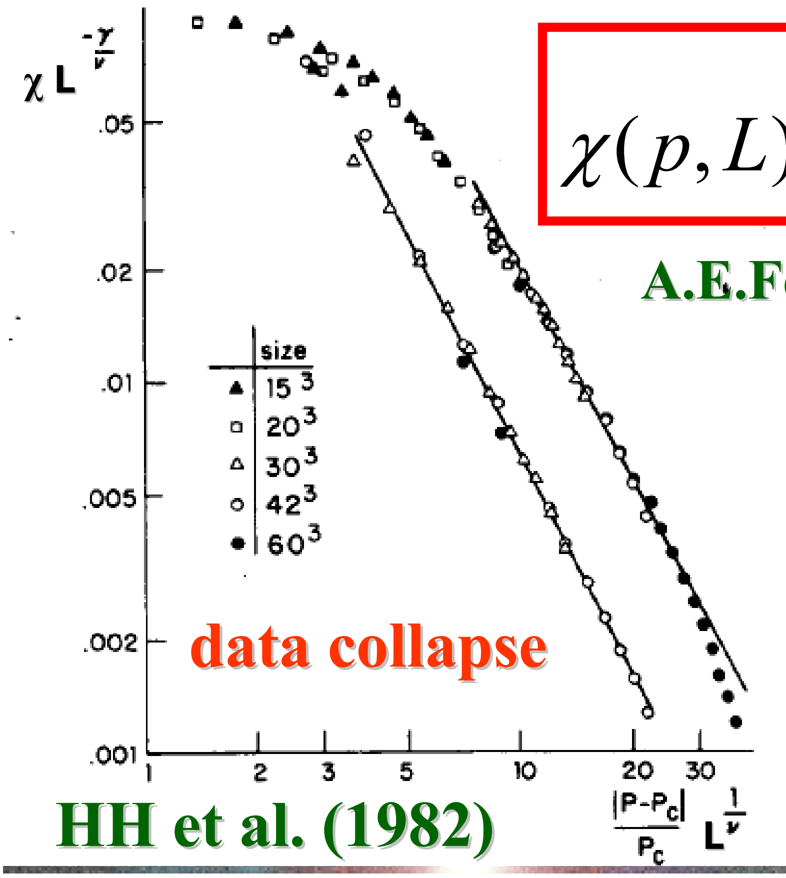
Apply finite size scaling

Extrapolation to infinite size



$$p_{eff}(L) = p_c(1 - aL^{-\frac{1}{\nu}})$$

Finite size scaling for χ



HH et al. (1982)

$$\chi(p,L) = L^{\frac{\gamma}{\nu}} \aleph_{\chi}[(p-p_c)L^{\frac{1}{\nu}}]$$

A.E.Ferdinand and M.E Fisher (1967)

at p_c:

$$\chi_{\max}(L) \propto L^{\frac{\gamma}{\nu}}$$

Finite size scaling of OP

fraction of sites in spanning cluster (OP): $\boxed{P \propto (p-p_c)^{\beta}}$

finite size scaling: $$\boxed{P(p,L) = L^{-\frac{\beta}{\nu}} \aleph_P[(p-p_c)L^{\frac{1}{\nu}}]}$$

at p_c: $\boxed{P \propto L^{-\frac{\beta}{\nu}}}$ $\boxed{M_\infty \propto L^{d_f}}$

$$\boxed{M_\infty \propto PL^d \propto L^{-\frac{\beta}{\nu}+d} \propto L^{d_f}}$$

fractal dimension: $\boxed{d_f = d - \frac{\beta}{\nu}}$

Fractal dimension of IIC

at p_c:

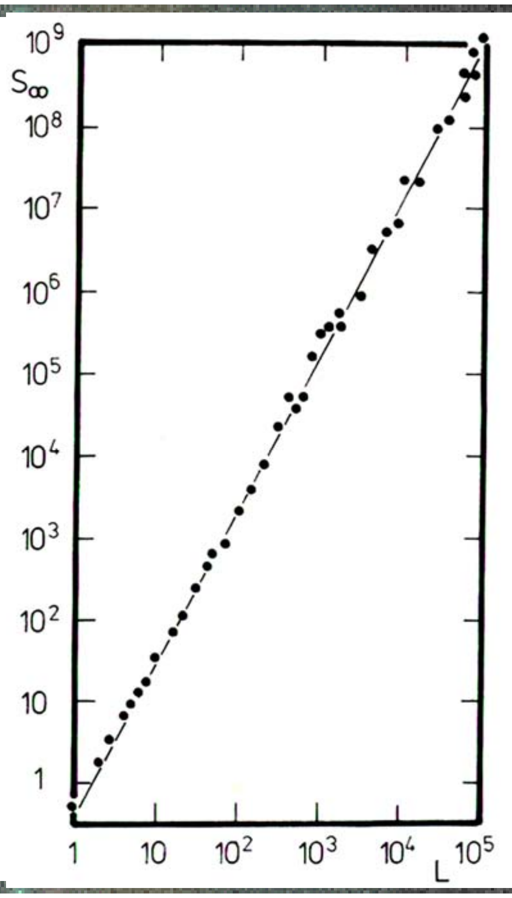
incipient infinite cluster (IIC)

$$\boxed{M_\infty \equiv PL^d \propto L^{d_f}}$$

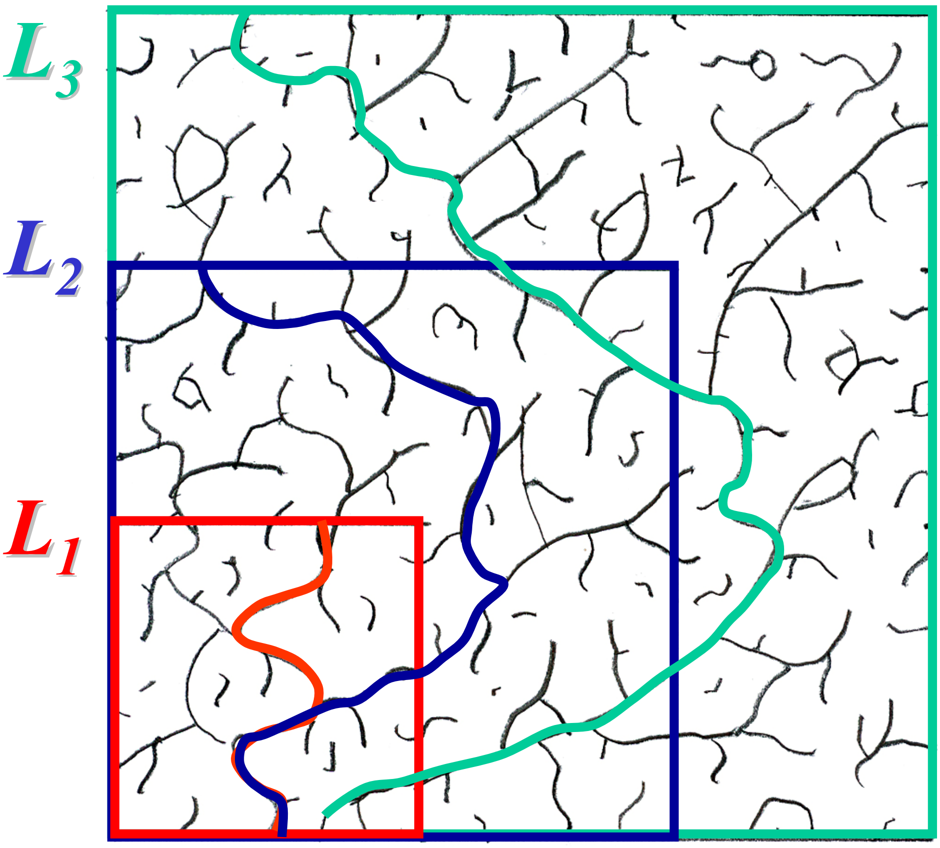
$d_f = 91/48$ in $d = 2$

$d_f \approx 2.51$ in $d = 3$

$$\boxed{d_f = d - \frac{\beta}{\nu}}$$

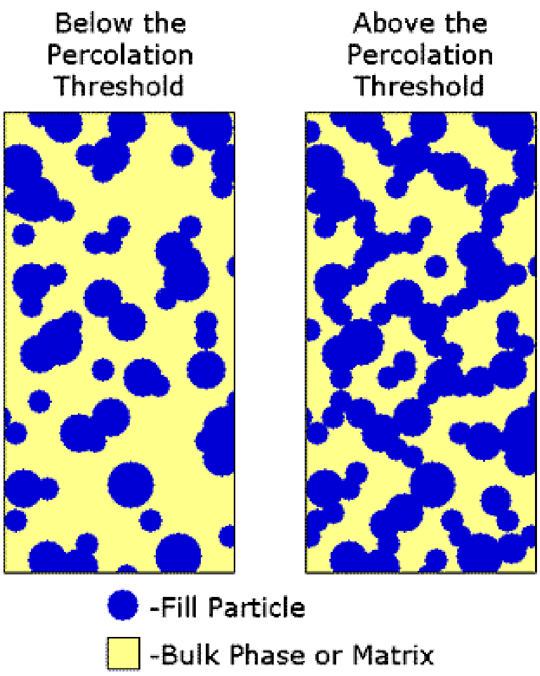


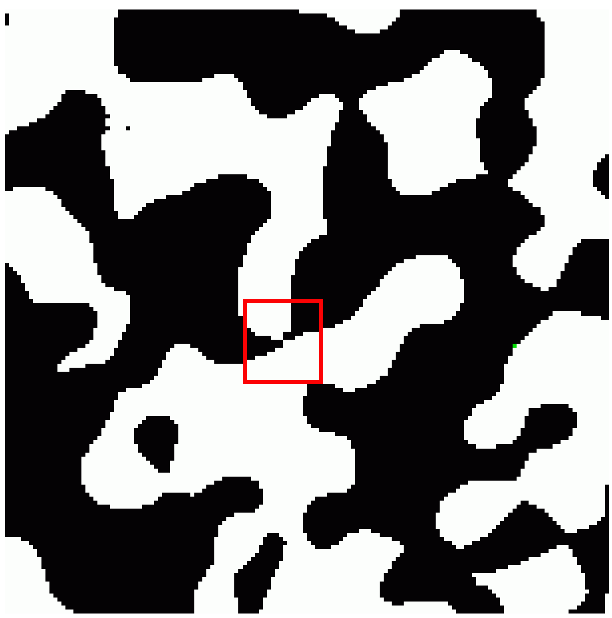
Volatile fractal



Continuum percolation

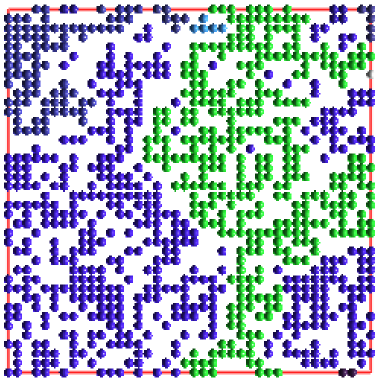
Swiss cheese model

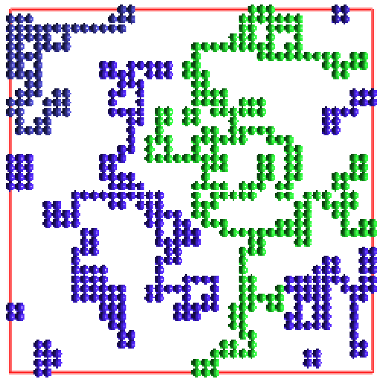




Continuum

Bootstrap percolation

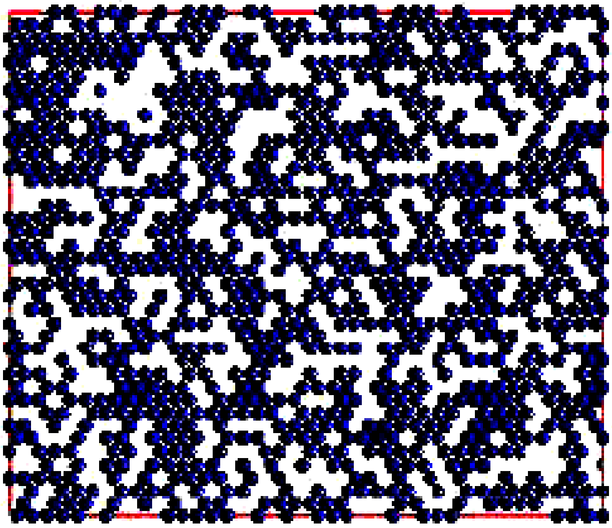




Start with $p = 0.55$ on square lattice.

Remove iteratively all sites that have less than m =2 neighbors: „culling“.

Bootstrap percolation



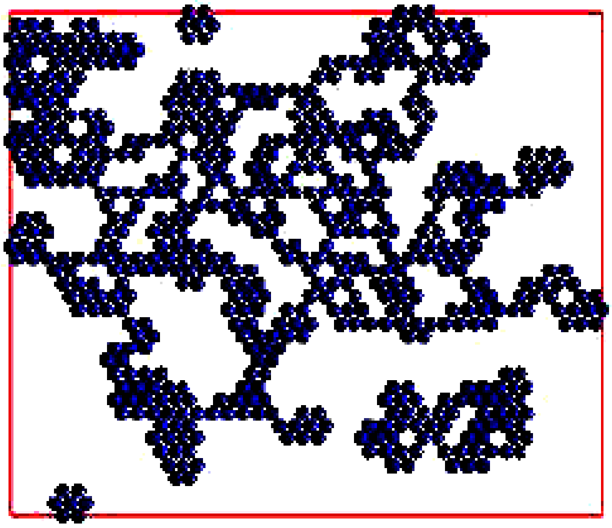


Figure 2. The initial freshly occupied lattice shown on the left for $m = 3$ on the triangular lattice at an initial concentration of $p = 0.66$, above the usual percolation threshold of $p_c = 1/2$ for this lattice. For initial occupation there is indeed an infinite cluster, but after culling there is a more compact cluster that does not percolate, as shown on the right.

triangular lattice, $m = 3$

Cellular Automata (CA)

John von Neuman and Stanislaw Ulam after 1940

discrete determinstic dynamics

discrete = { Boolean variables; on a lattice; from t to t+1 }

References to CA

- Stephen Wolfram: „Cellular Automata and Complexity“ (Perseus, 1994)
- S. Wolfram: „A New Kind of Science“ (Wolfram Media, 2002)
- A. Ilachinski: „Cellular Automata“ (World Scientific Publ., 2001)
- B. Chopard: „Cellular Automata Modelling of Physical Systems“ (Cambridge University Press, 2005)

Definition of CA

σ_i binary variable on site i of a graph

rule: $$\boxed{\sigma_i(t+1) = f_i\left(\sigma_j(t),\, j = 1, \ldots, k\right)}$$

k = number of inputs

There exist 2^{2^k} **possible rules.**

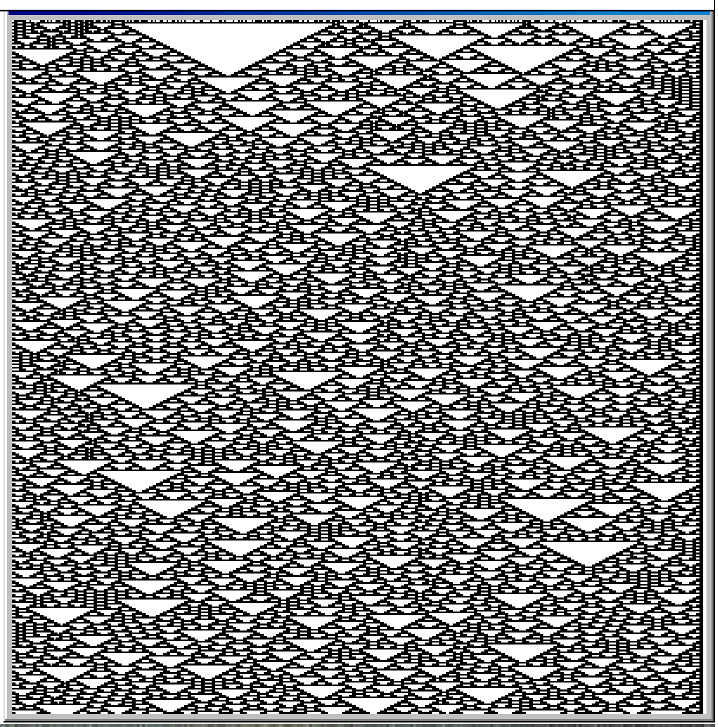
Time evolution

example:

entries:	111	110	101	100	011	010	001	000
$f(n)$:	0	0	0	1	1	1	1	0

On every site of a one-dimensional chain we put the same rule f with $k = 3$ inputs, namely the site itself and its two nearest neighbors and put at $t = 0$ a random configuration of bits.

time



„ rule 30“

Classification of CA

ETH

$$k = 3$$

entries:	111	110	101	100	011	010	001	000
$f(n)$:	0	1	1	0	0	1	0	1

$$f(n) = 64 + 32 + 4 + 1 = 101$$

$$c = \sum_{n=0}^{2^k - 1} 2^n f(n)$$

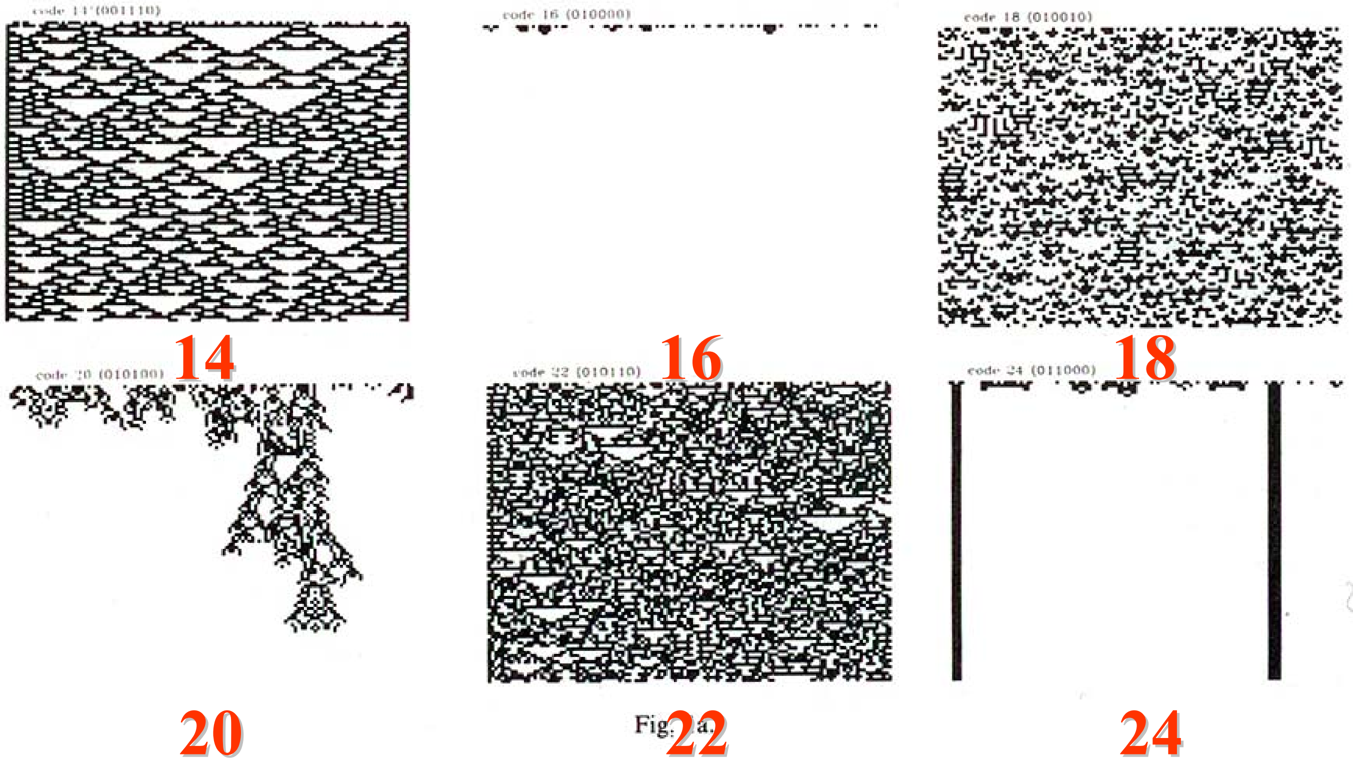
Examples for $k = 3$

ETH

entries:	111	110	101	100	011	010	001	000
4 :	0	0	0	0	0	1	0	0
8 :	0	0	0	0	1	0	0	0
20:	0	0	0	1	0	1	0	0
28;	0	0	0	1	1	1	0	0
90:	0	1	0	1	1	0	1	0

applet

Evolution of different rules



Classes of Automata
(Wolfram)

Damage spreading

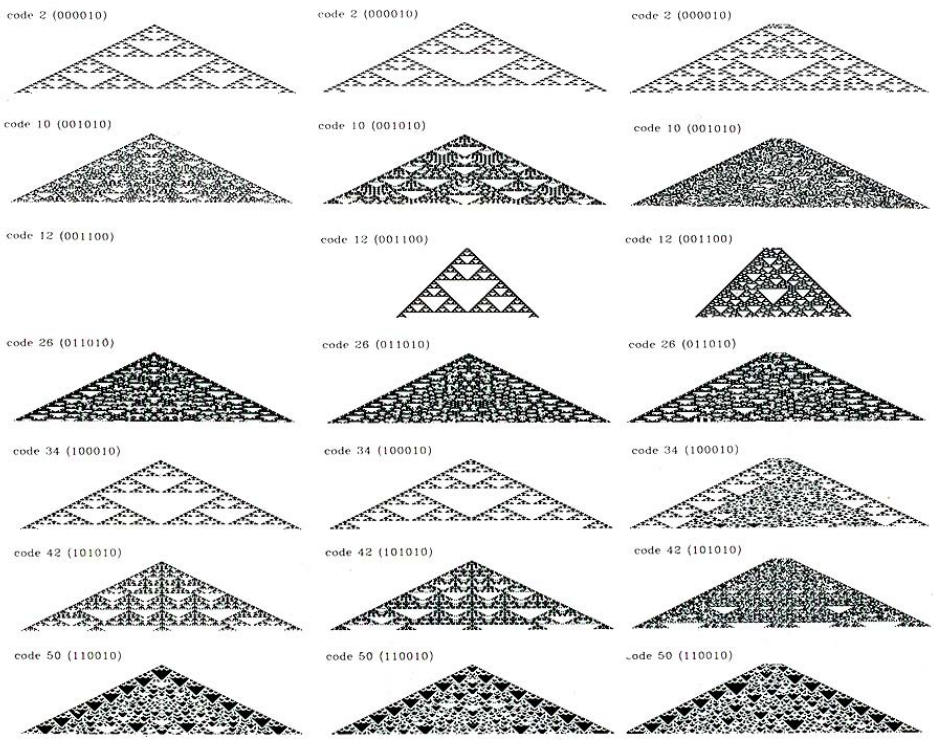


Fig. 9. Evolution of some class 3 totalistic cellular automata with $k = 2$ and $r = 2$ (as illustrated in fig. 1) from initial states containing one or a few nonzero sites. Some cases yield asymptotically self-similar patterns, while others are seen to give irregular patterns.

The Game of Life

J.H. Conway (1970)

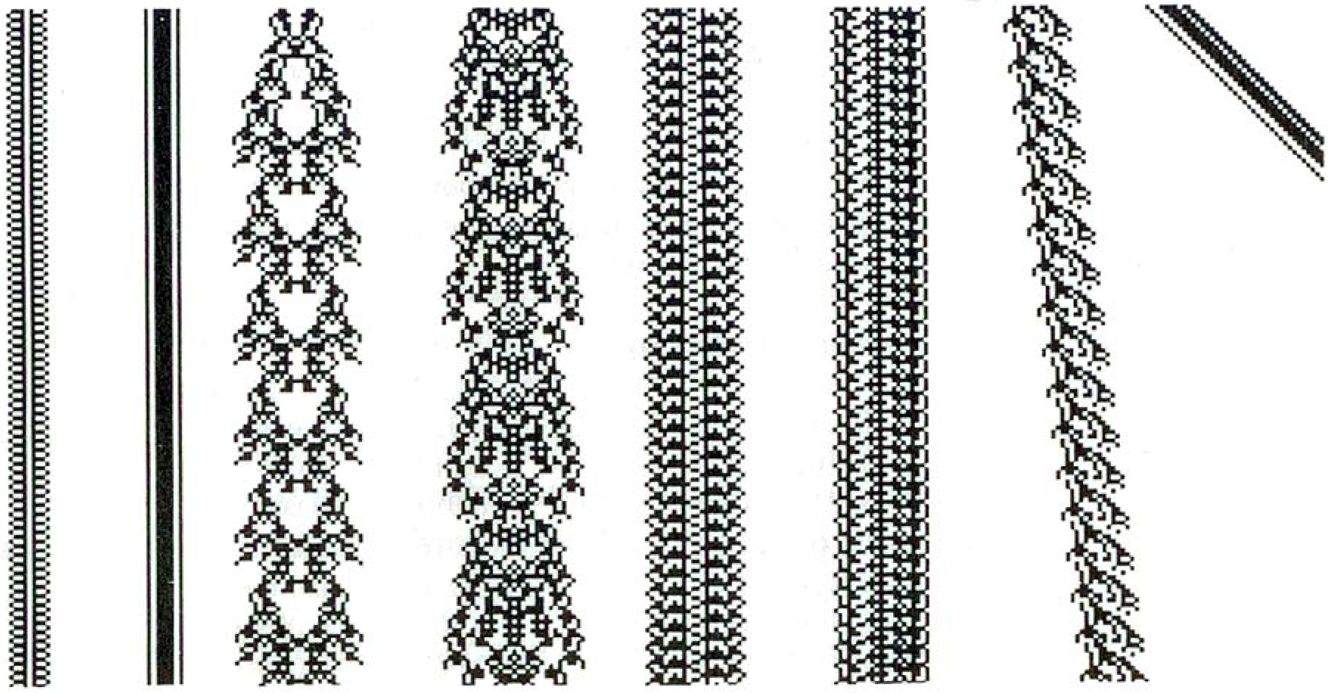
Consider a square lattice. Be n the number nearest and next-nearest neighbors that are „1“.

rule:

- $n < 2 \Rightarrow 0$
- $n = 2 \Rightarrow$ stay as before
- $n = 3 \Rightarrow 1$
- $n > 3 \Rightarrow 0$

The Game of Life

gliders:



The Game of Life

glider gun: