993SM - Laboratory of Computational Physics Unit XI - II part December 6, 2024

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Modelling other random processes

- Fractals & Diffusion Limited Aggregates
- Percolation

Diffusion Limited Aggregation

Several examples of formation of natural patterns showing common features:

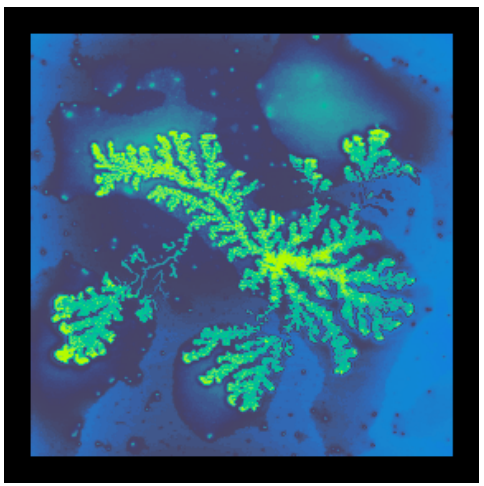
Electrodeposition:
cluster grown from a copper sulfate solution in an electrodeposition cell

Dielectric breakdown:
High voltage dielectric breakdown within a block of plexiglas

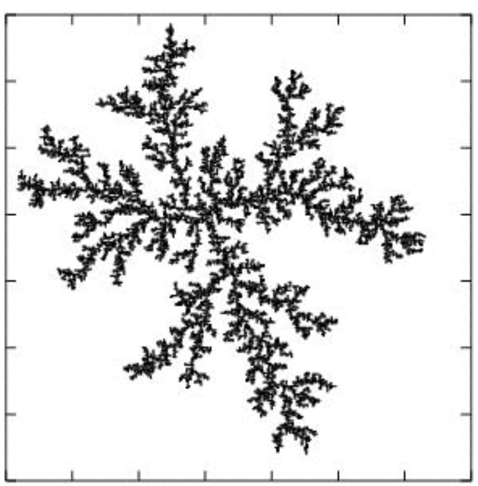
These common features that can be captured by very simple models:

Diffusion Limited Aggregation

- simple model of FRACTALS GROWTH, initially proposed for irreversible colloidal aggregation, although it was quickly realized that the model is very widely applicable.
- by T.A. Witten and L.M. Sander, Phys. Rev. Lett. 47, 1400 (1981)



REAL IMAGE (Atomic Field Microscopy) of a gold colloid of about 15 nm over a gel substrate



SIMULATION

DLA: algorithm

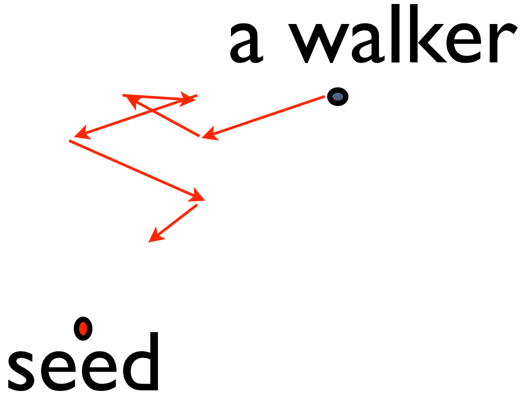
* Start with an immobile seed on the plane

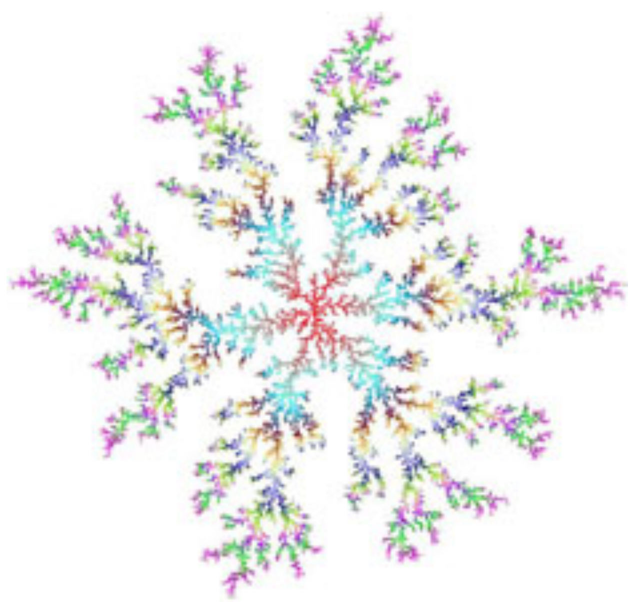
* A walker is then launched from a random position far away and is allowed to diffuse

* If it touches the seed, it is immobilized instantly and becomes part of the aggregate

* We then launch similar walkers one-by-one and each of them stops upon hitting the cluster

* After launching a few hundred particles, a cluster with intricate branch structures results

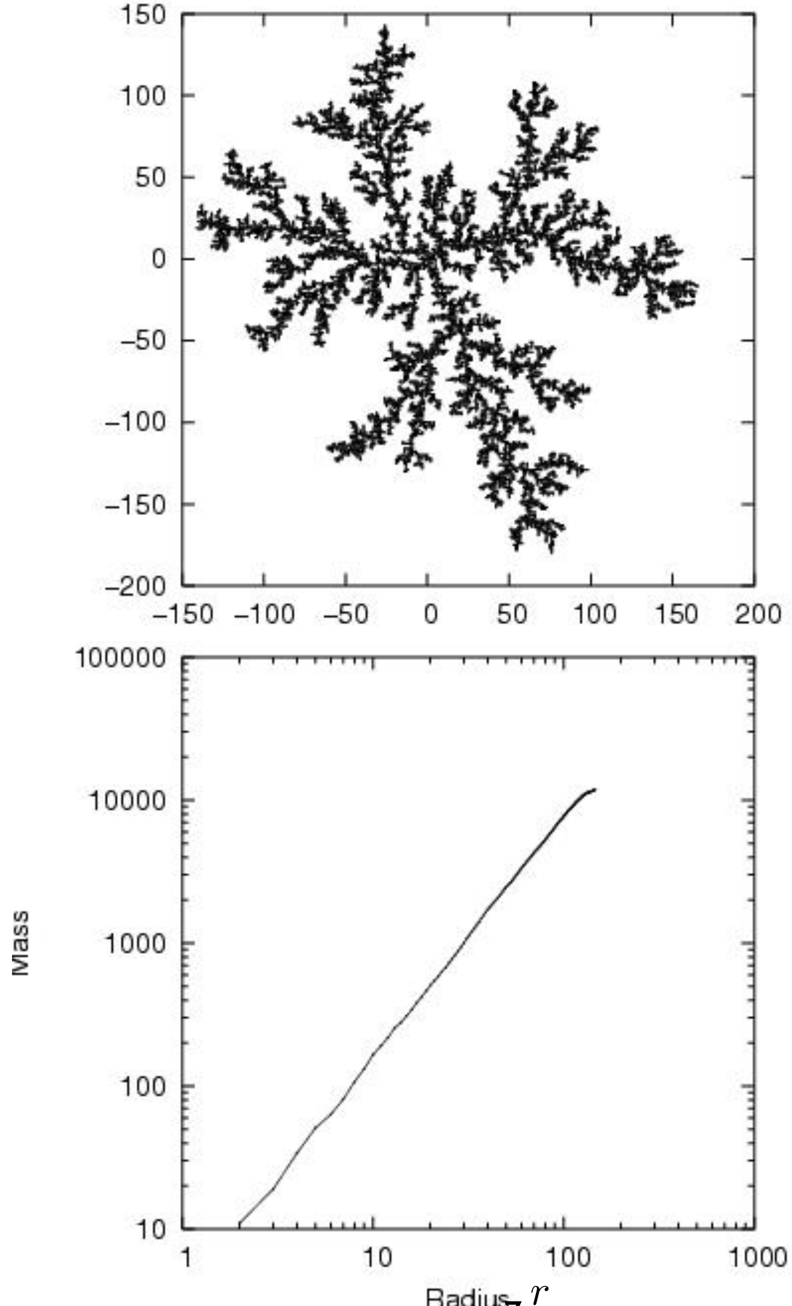




DLA: algorithm - details

- We launch walkers from a “launching circle” which inscribes the cluster
- They are discarded if they wander too far and go beyond a “killing circle”
- The diffusion is simulated by successive displacements in independent random directions
- At every step, the walker which would aggregate is checked to detect any overlapping with the particles on the cluster

DLA: results



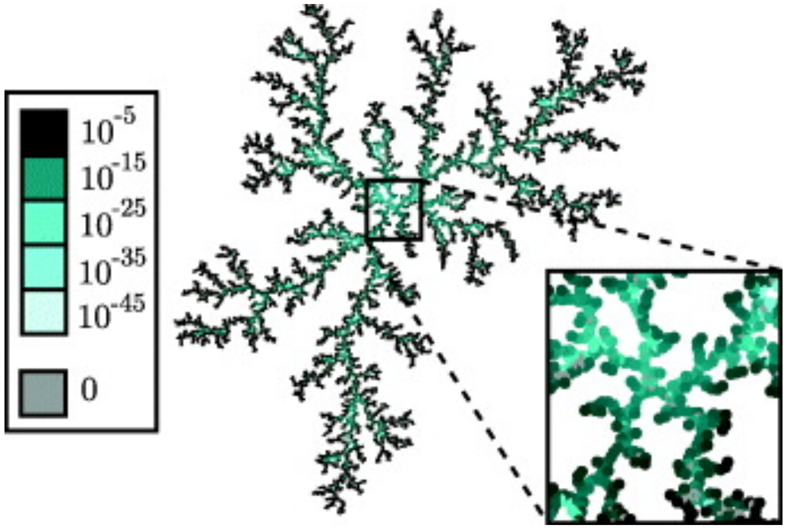
(mass M of the cluster ≡ number of particles N)

$$\ln N \propto \ln r$$
$$\Downarrow$$
$$N \propto r^k$$

DLA: interesting quantities

- in a "normal" 2D object: $N \propto r^2$
- FRACTAL DIMENSION: the number of particles N with respect to the maximum distance r of a particle of the cluster from its center of mass is $N \propto r^{D_f}$, with

$1 < D_f < 2$

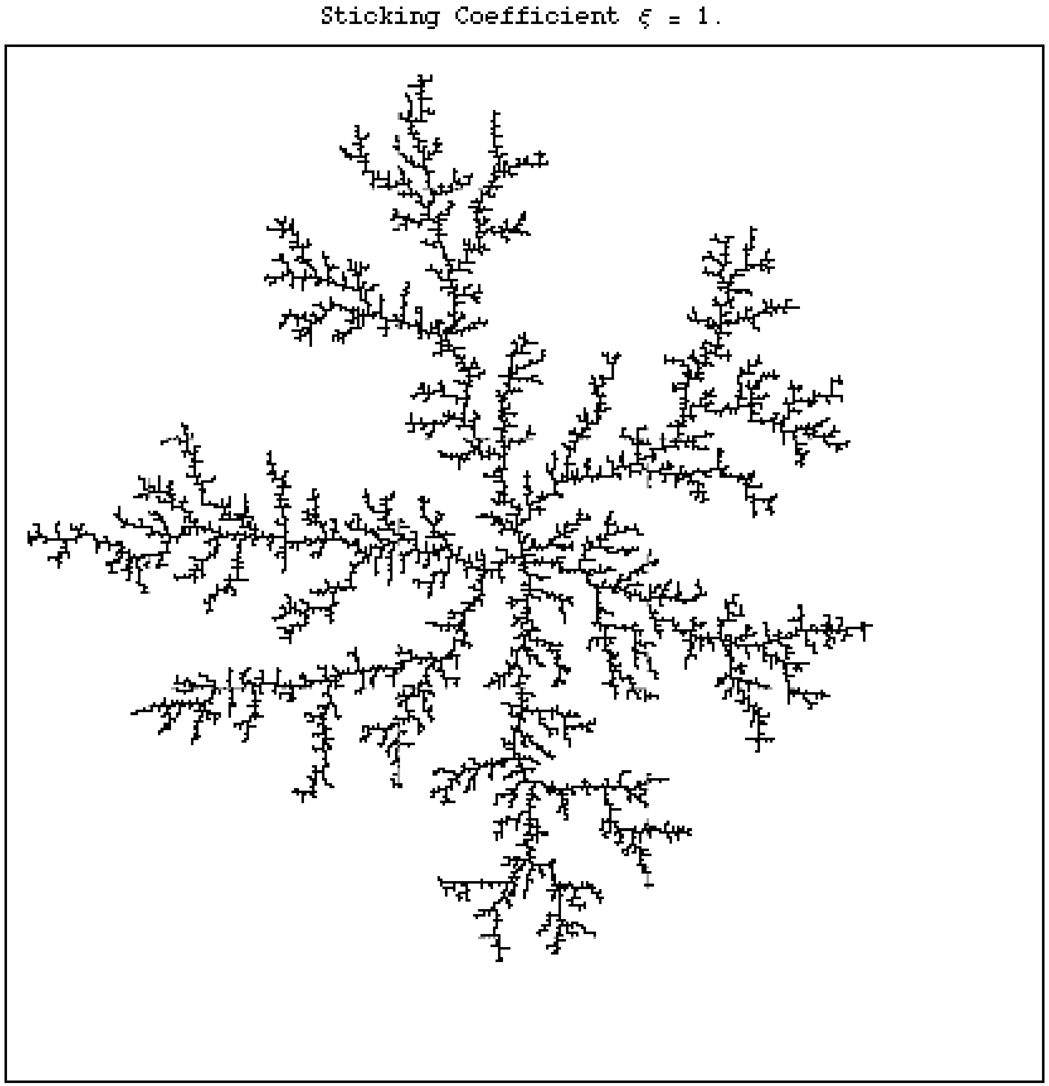


DLA: algorithm - details II

- the simplest DLA models: diffusion on a lattice. On a **square lattice**, 4 adjacent sites are available for the diffusing particle to stick
- modification: the particle will stick with certain probability (the "sticking coefficient") - to simulate somehow the surface tension
- another modification: with a sort of Brownian diffusion in the continuum

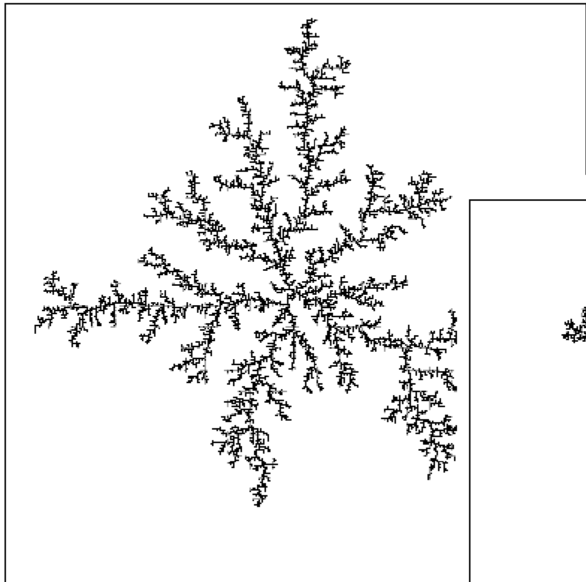
DLA: results

$$1 < D_f = 1.6 < 2$$

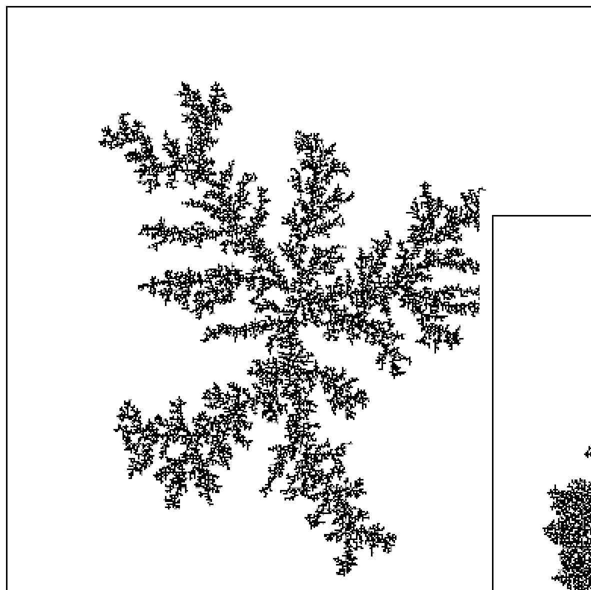


DLA: results

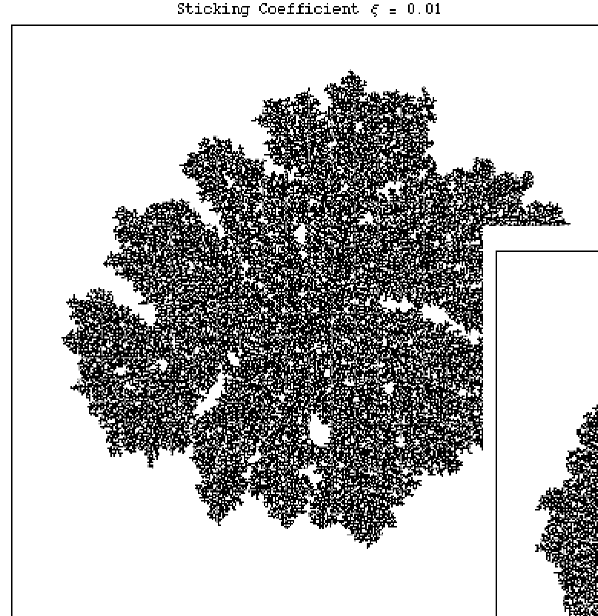
Sticking Coefficient ξ = 0.5



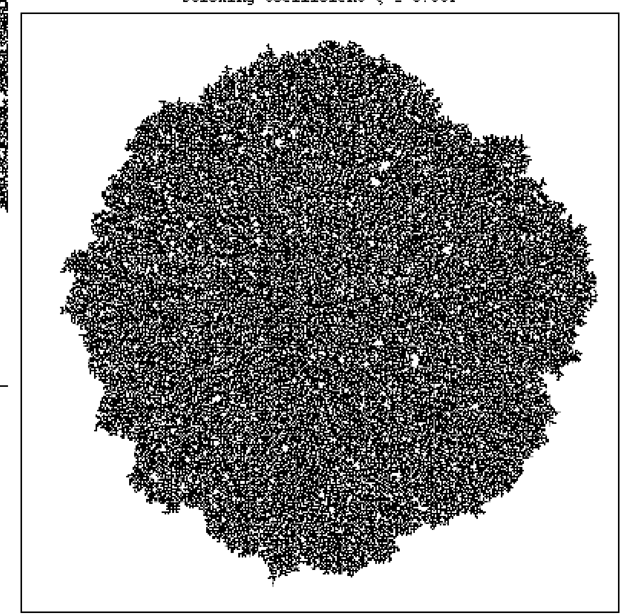
Sticking Coefficient ξ = 0.1



Sticking Coefficient ξ = 0.01



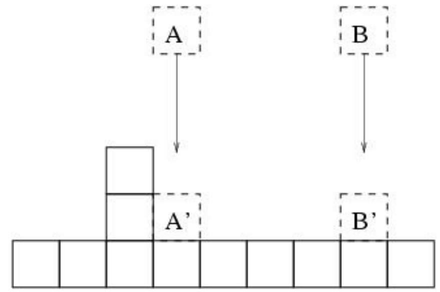
Sticking Coefficient ξ = 0.001

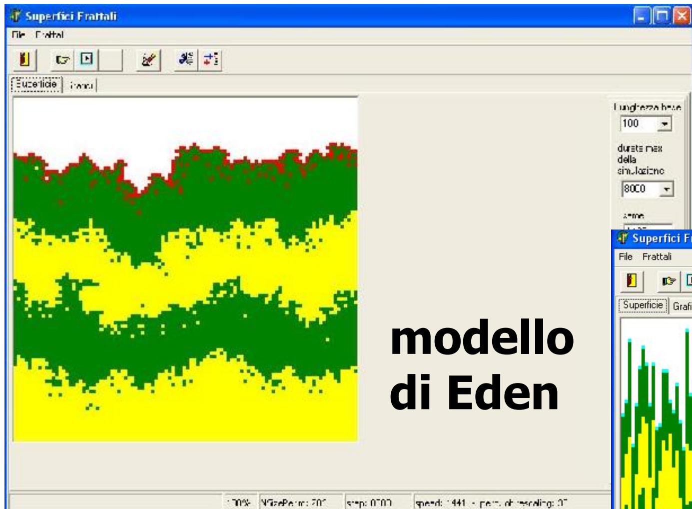


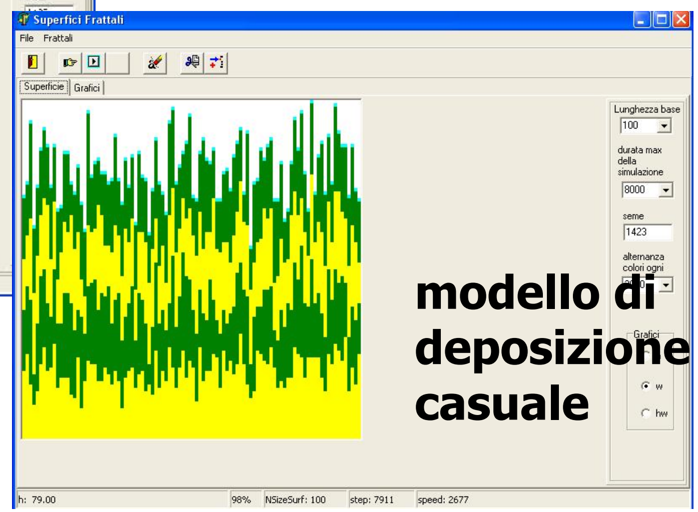
$$D_f \to 2$$

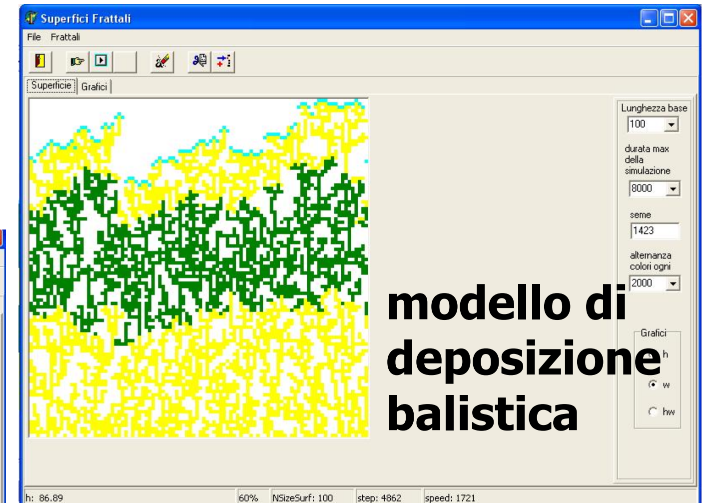
as the sticking coeff. $\to 0$

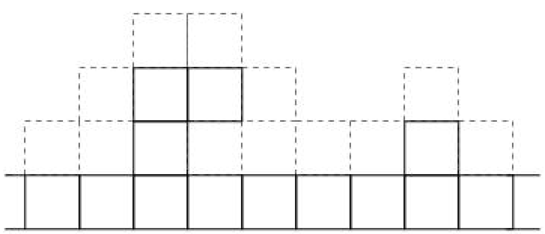
Models of surface growth

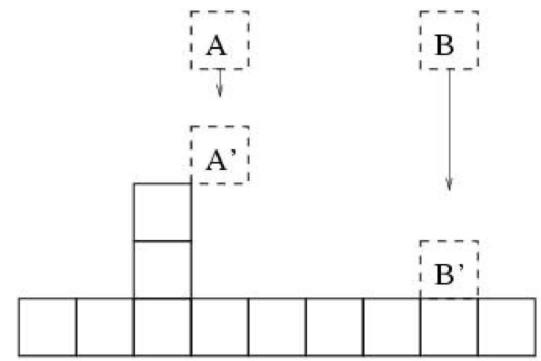












see e.g. Barabasi & Stanley, ***Fractal concepts in surface growth***, Cambridge University Press

Models of surface growth

The Eden model - algorithm:

(a) choose randomly a lattice site and occupy it. The *nearest neighbor sites* of the occupied site (i.e. 4 sites in case of a square lattice) are the *perimetral sites*.

(b) choose randomly a *perimetral site* and occupy it. When occupied, it is no longer a *perimetral site*: update the list of *perimetral sites* with the new ones. Repeat from (1).

Interesting quantities:

Average height: $$\bar{h} = \frac{1}{N_s}\sum_{i=1}^{N_s} h_i$$

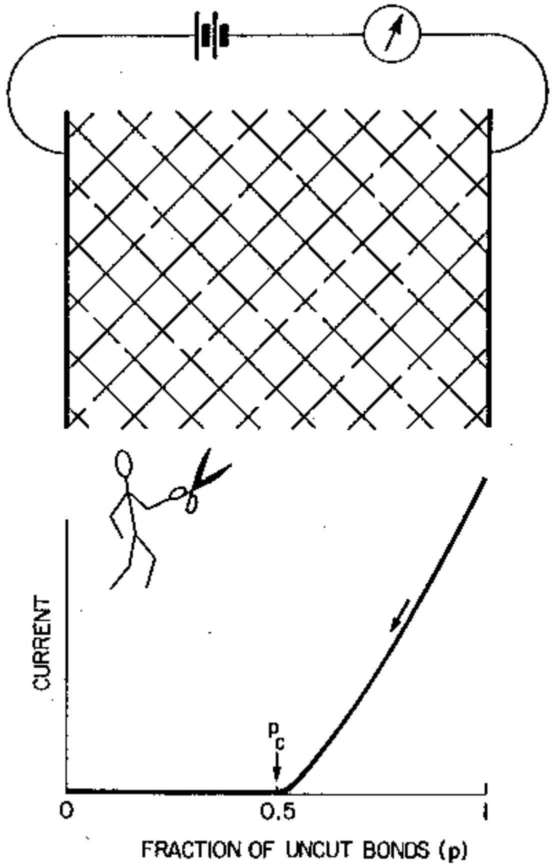
Roughness: $$w^2 = \frac{1}{N_s}\sum_{i=1}^{N_s}(h_i - \bar{h})^2,$$

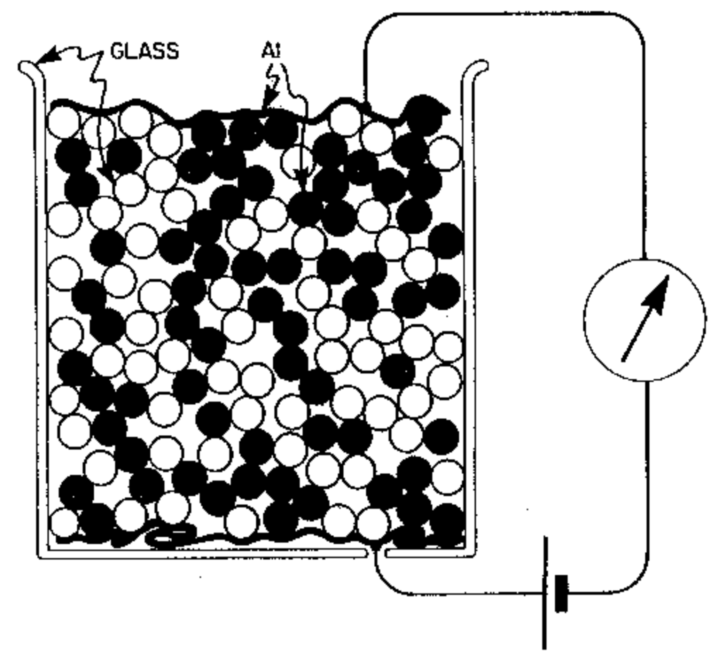
Modelling other random processes

- Fractals & Diffusion Limited Aggregates
- Percolation
- Monte Carlo approach for classical fluids

Percolation

geometric connectivity in a stochastic system;
modeling threshold and transition phenomena



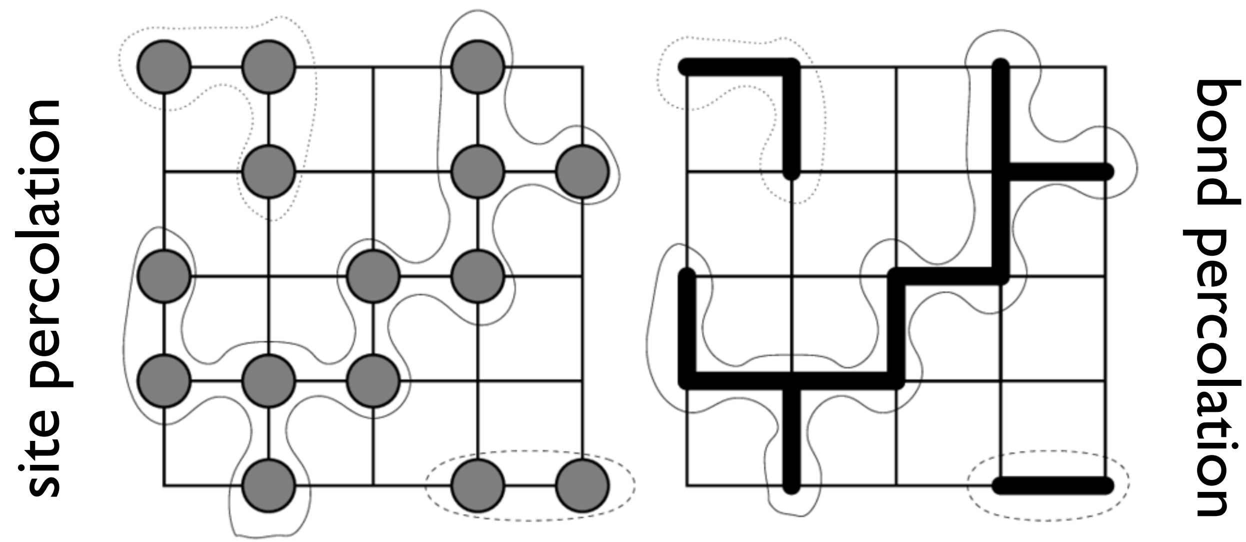


existence of a critical occupation fraction P_c above which spanning clusters occur (in nature: mixtures of conducting/insulating spheres...; resistor networks..)

Percolation

- metal/insulator threshold behavior in resistor networks (discrete percolation) and in alloys (continuous percolation)

Other examples:
- fluid adsorption in a porous medium
- spreading of a disease in a population
- spreading of a forest fire...
- liquid/glass transition...
- ...



By Rudolf A. Römer

Percolation

Definitions:

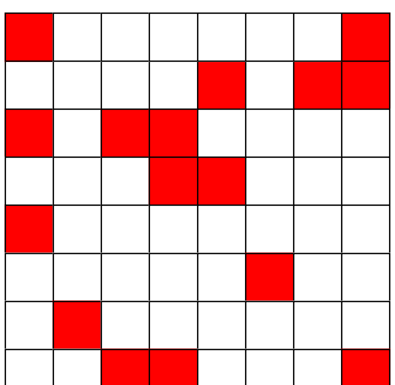
p: occupation probability of each identity (site, bond)

Cluster: group of identities (sites, bonds,...) connected by nearest neighboring bonds

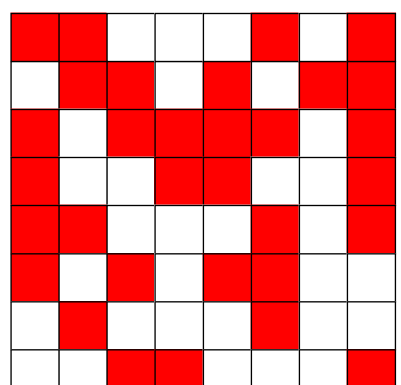
Percolating clusters: connecting two boundaries

which is the critical percolation threshold p_c ?

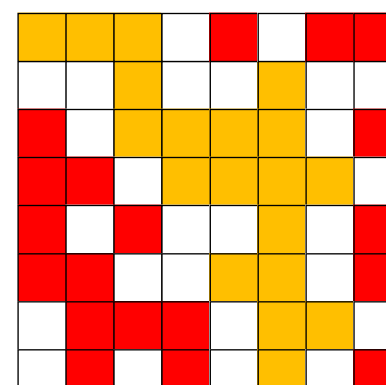
Example of site percolation on a lattice:



L = 8 p = 0.25



L = 8 p = 0.50

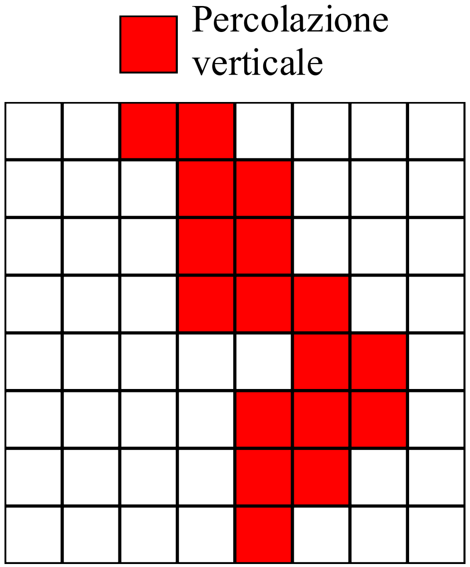


L = 8 p = 0.60

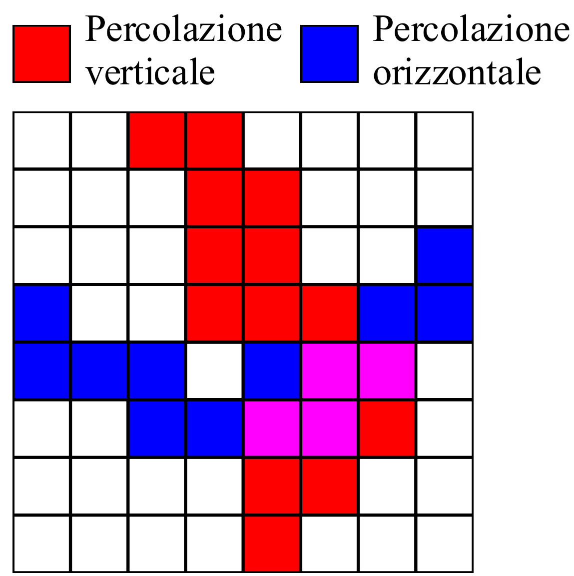
Percolation threshold

p_c depends on the criteria (different possibilities):

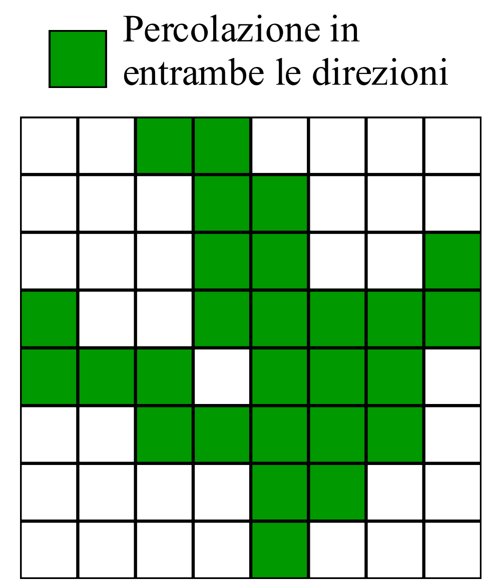
Connection along one fixed direction



Connection along one (any, horizontal or vertical) direction



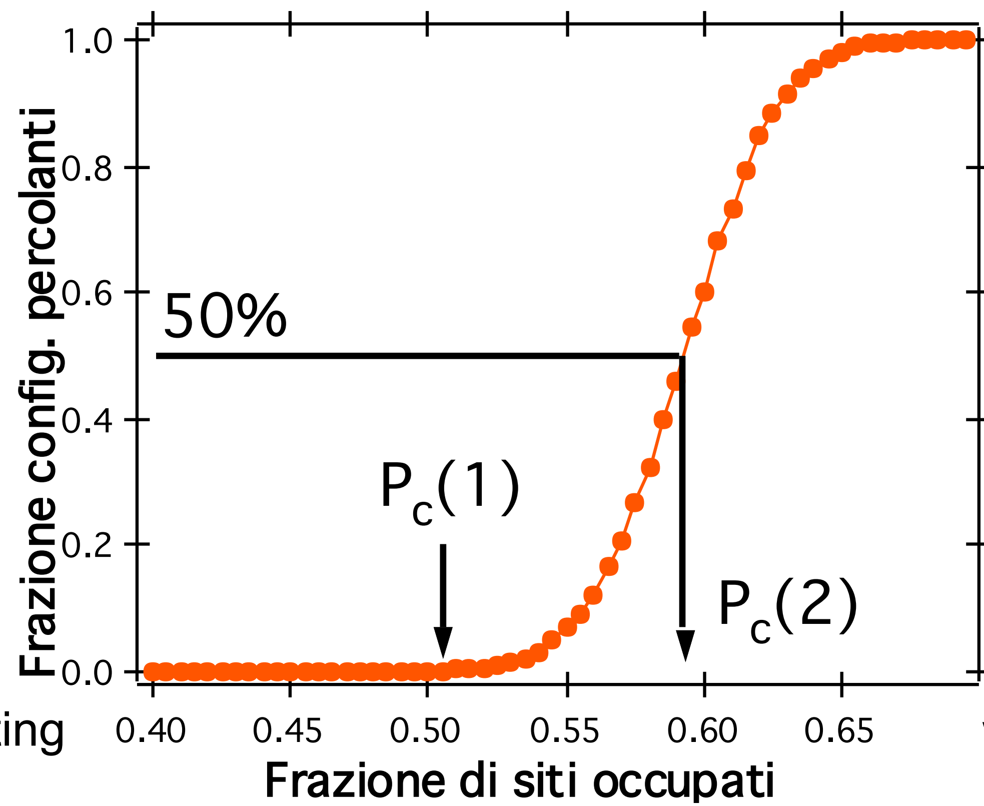
Connection in all directions



Percolation threshold

p_c depends on the criteria (different possible):

$P_c(1)$:
fraction of occupied sites when the first percolating cluster is established



$P_c(2)$:
fraction of occupied sites when 50% of the clusters are percolating

$$P_C(1) \equiv P_C(2) \qquad \text{for} \qquad L \to \infty$$

Monte Carlo approach

fix **L** => Lattice description

fix **p** => Site (or bond) filling accordingly

Identification and characterization of the clusters

```
do i,j=1,L
    r(i,j)=random(seed)
    if r(i,j) < p then index (i,j) = -1
    if r(i,j) > p then index (i,j) = 0
end do
```

use some algorithm
of cluster labelling to identify
the different clusters

generation of many configurations for each **p**

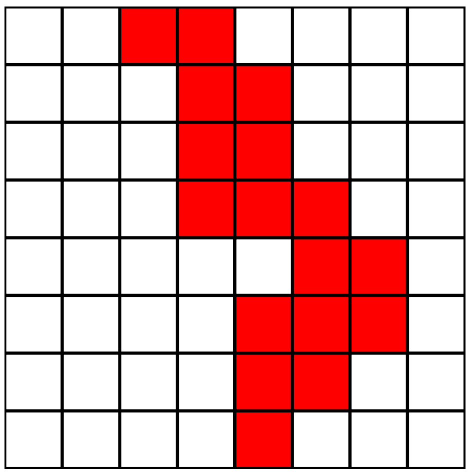
data analysis;
account for size effect (vary **L**)!

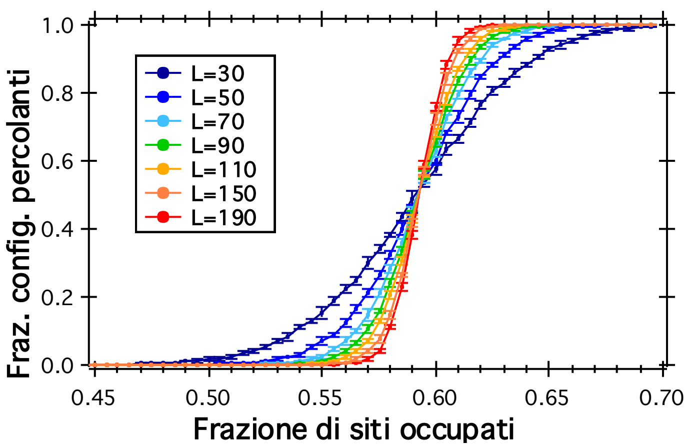
Results

for different percolation criteria and different size

Connection along one fixed direction

Percolazione verticale

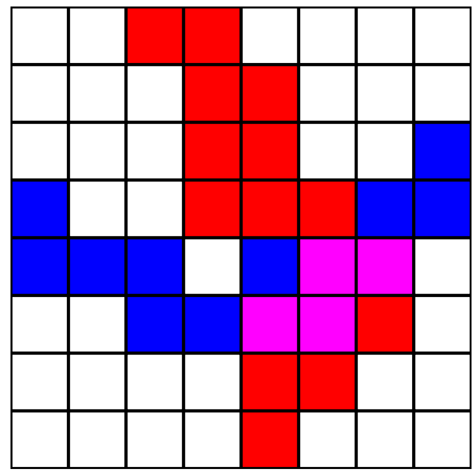


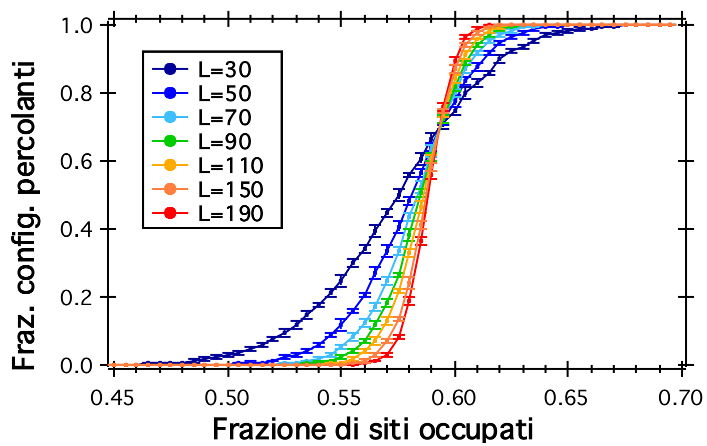


Connection along one (any, horizontal or vertical) direction

Percolazione verticale

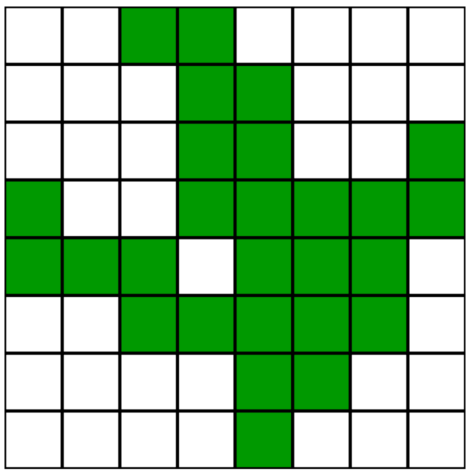
Percolazione orizzontale

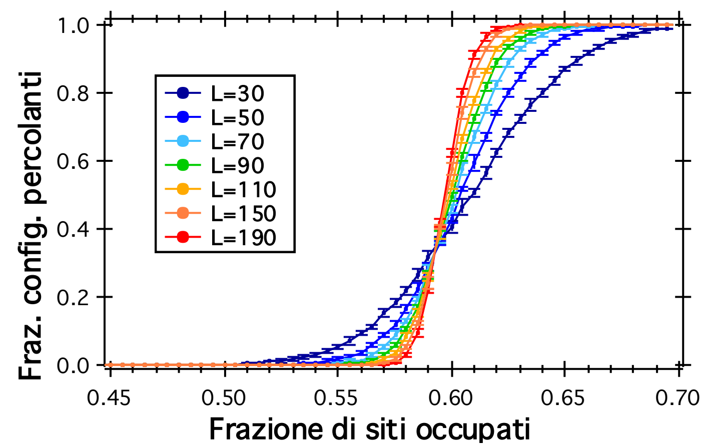




Connection in all directions

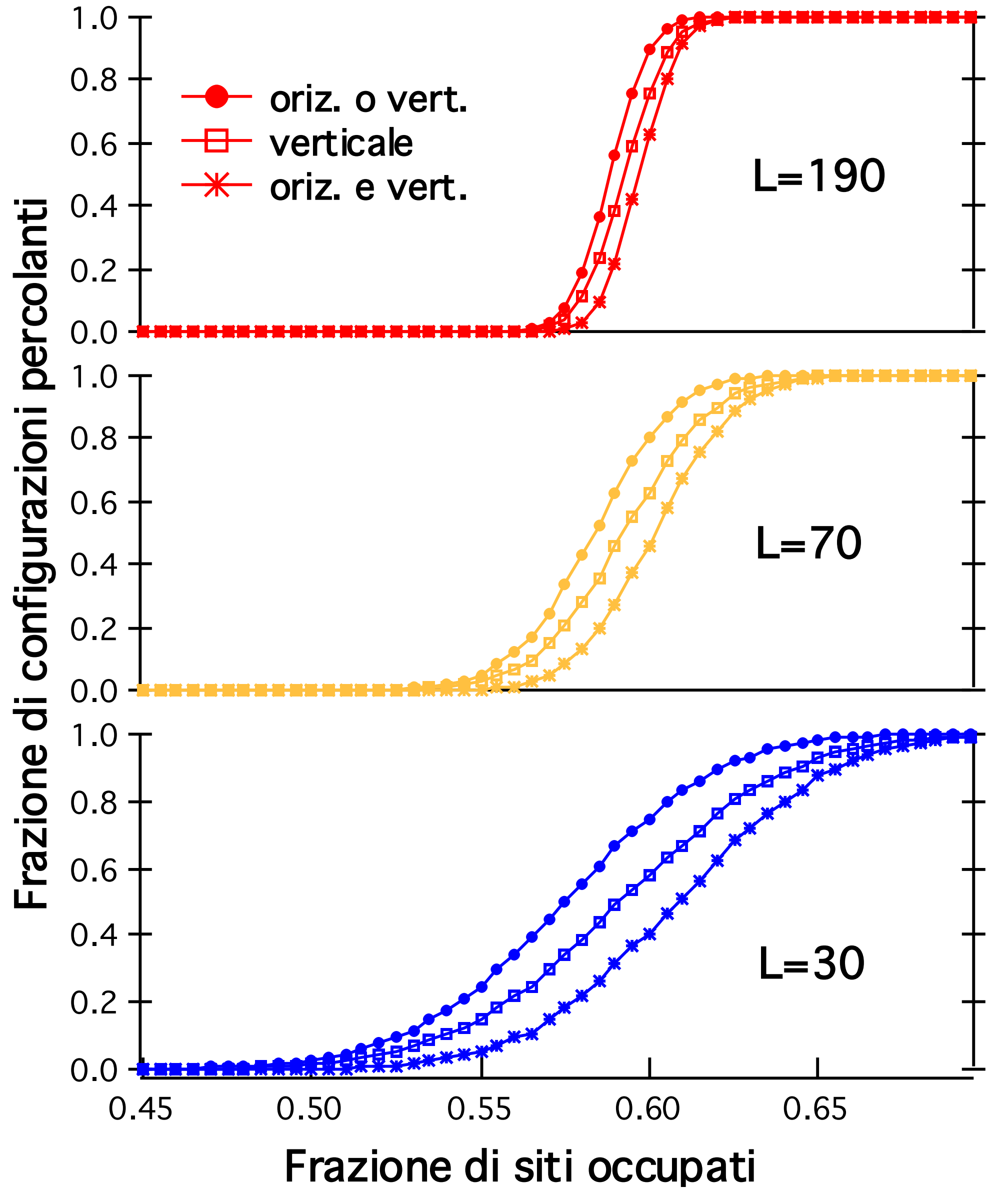
Percolazione in entrambe le direzioni





Results

for different percolation criteria and different size



Results
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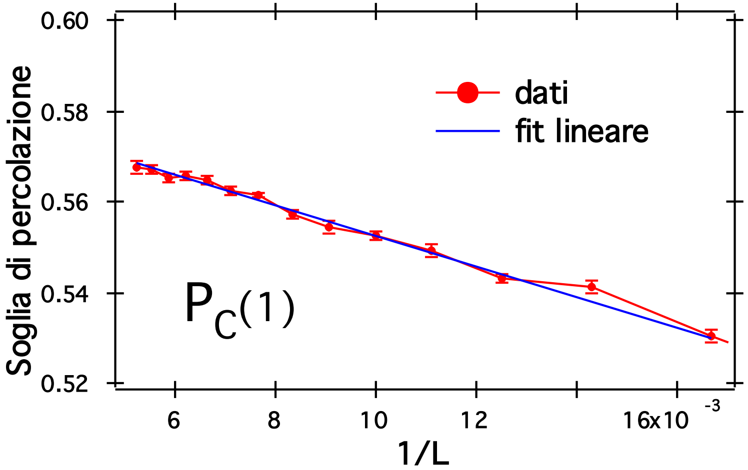
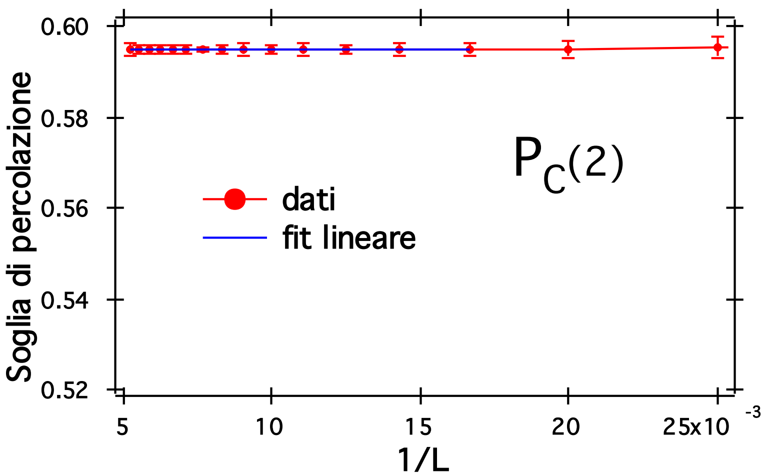


extrapolate the behavior for

$$L \to \infty$$

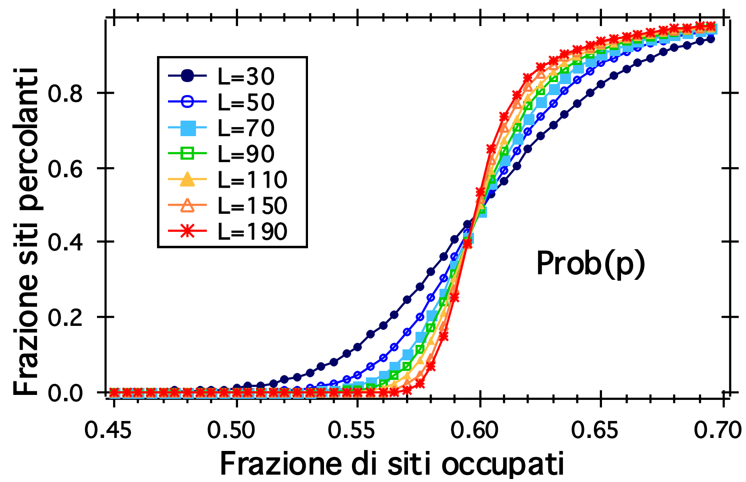
$$1/L \to 0$$



$$P_C^\infty(1) = P_C^\infty(2) = 0.59 \pm 0.05$$

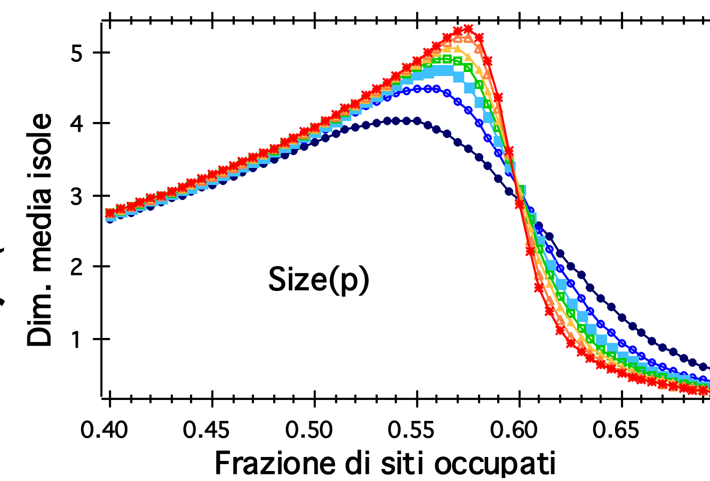
Results

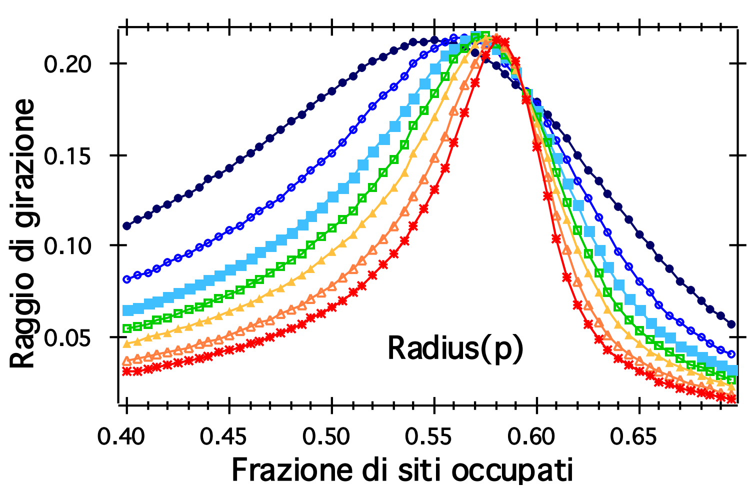
other interesting quantities



probability Prob(p) for a site to be included in a percolating cluster

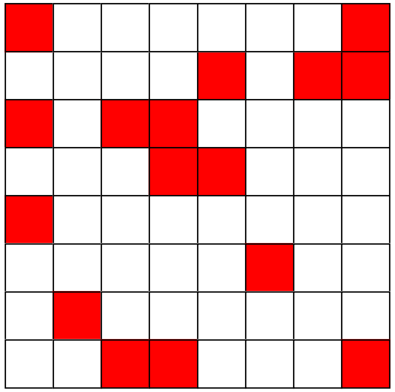
average size Size(p) of a non-percolating cluster





radius of gyration Radius(p) = $\sqrt{\frac{\sum_i^N (\vec{r}_i - \vec{r}_{cm})^2}{N}}$

Cluster labelling



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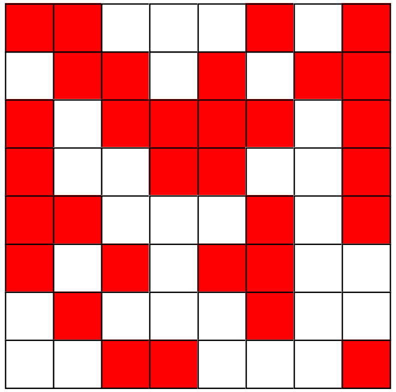
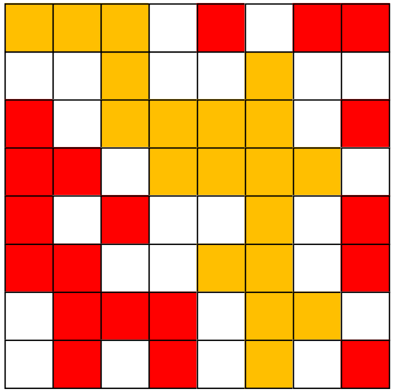


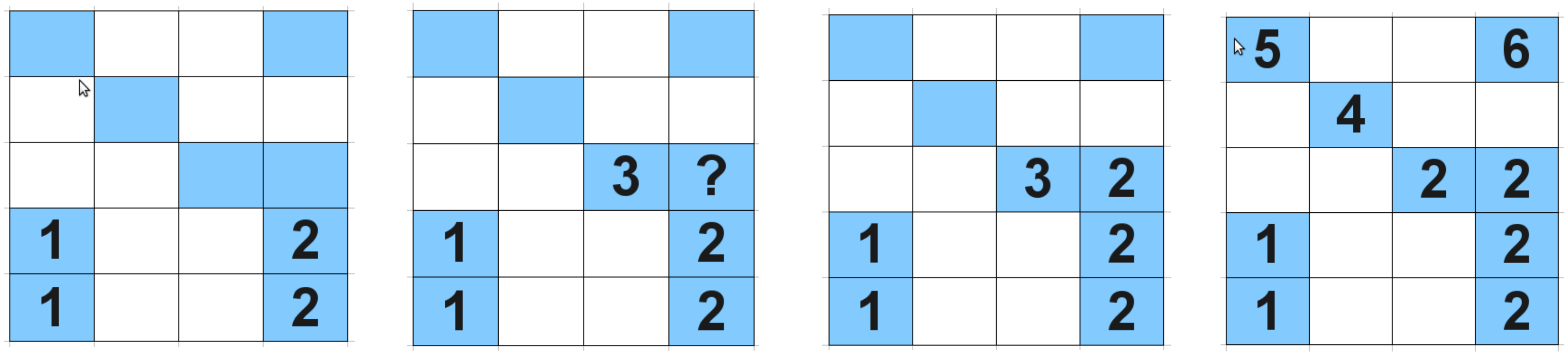
L = 8 p = 0.50



L = 8 p = 0.60

The (non trivial) part of the model:
choose a smart algorithm to identify and label the clusters made of adjacent occupied sites

Cluster labelling



(1): span all the cells
(here: left => right
and bottom => up)
and start labeling

(2): attribute the minimum cluster label
to cells neighboring to different clusters

(3): refine labeling

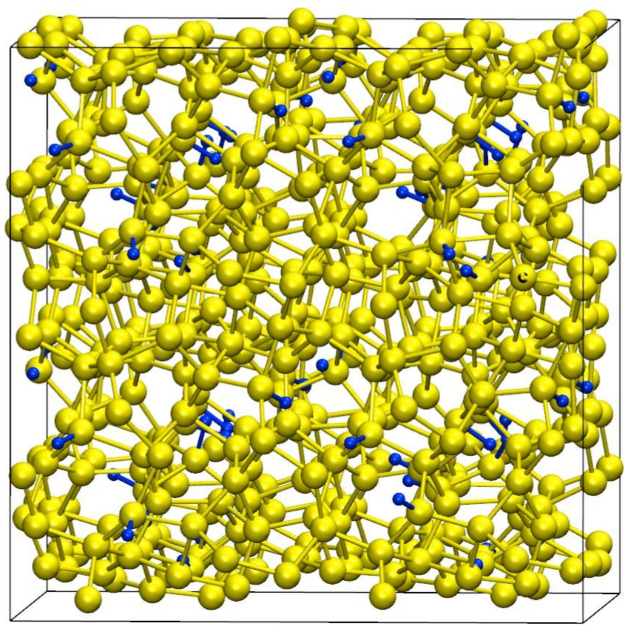
Hoshen- Kopelman algorithm for clusters labelling

Example of application in solid state physics

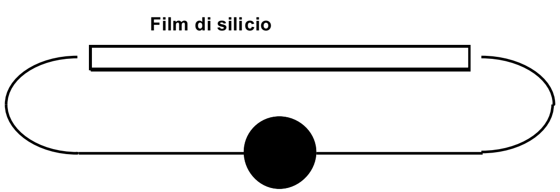
Dynamical Percolation Model of Conductance Fluctuations in Hydrogenated Amorphous Silicon

L.M. Lust e J. Kakalios, Phys. Rev. Lett. ***75,*** *11 (1995)*

Fluttuazioni di conduttività nel silicio amorfo idrogenato (*a*-Si:H) sono simulate utilizzando un modello dinamico di diffusione di resistenze in un reticolo in condizioni di soglia di percolazione. Una frazione di siti di reticolo è designata come una trappola tale per cui quando un resistore diffonde in una di esse, rimane localizzato per un periodo finito di tempo.

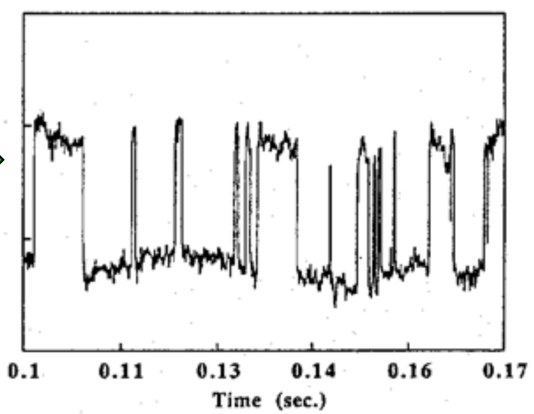


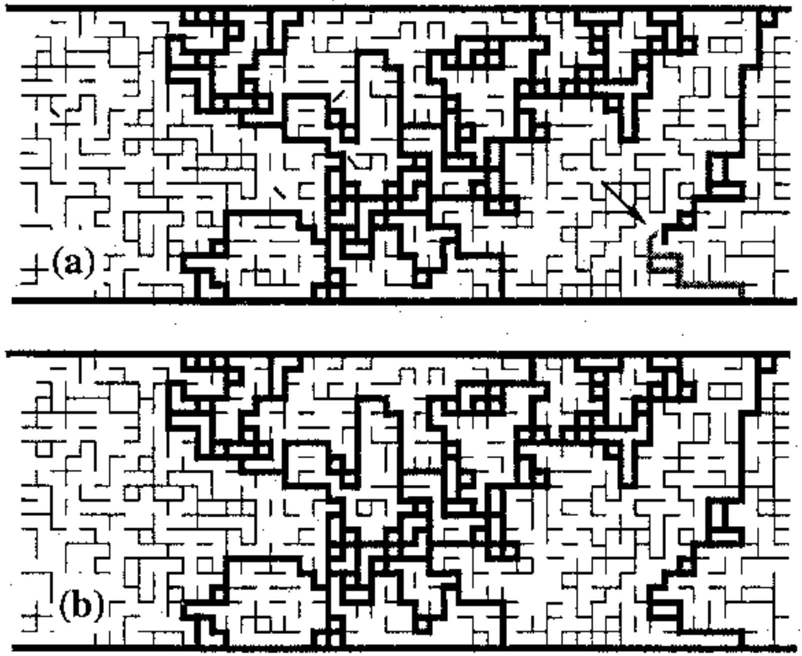
A model of a-Si:H from https://doi.org/10.1016/j.commatsci.2018.08.027



Fluttuazioni di tipo "telegrafico"

Fluttuazioni di conduttività misurate sperimentalmente

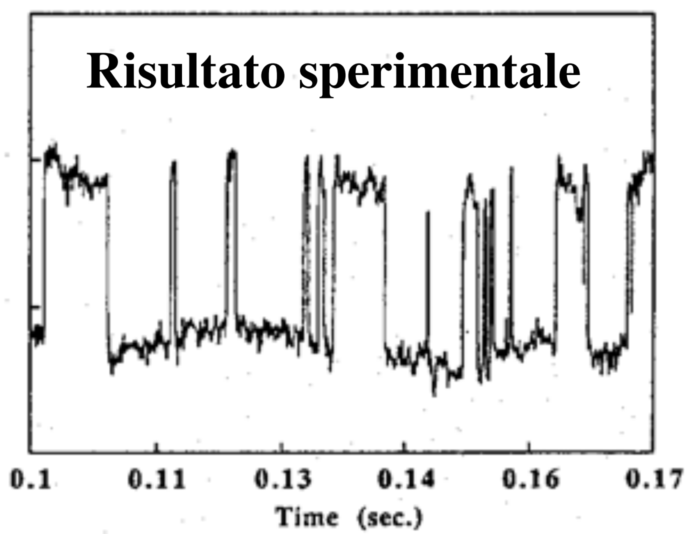


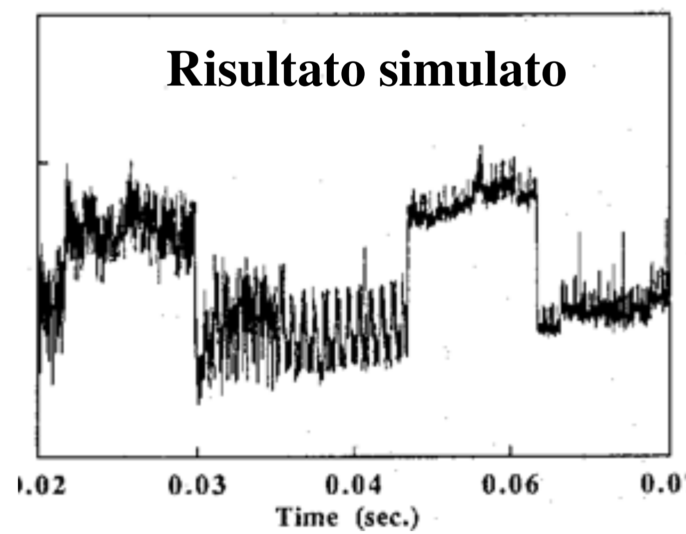


Rete casuale di resistenze con P ~ P_C (fisso)

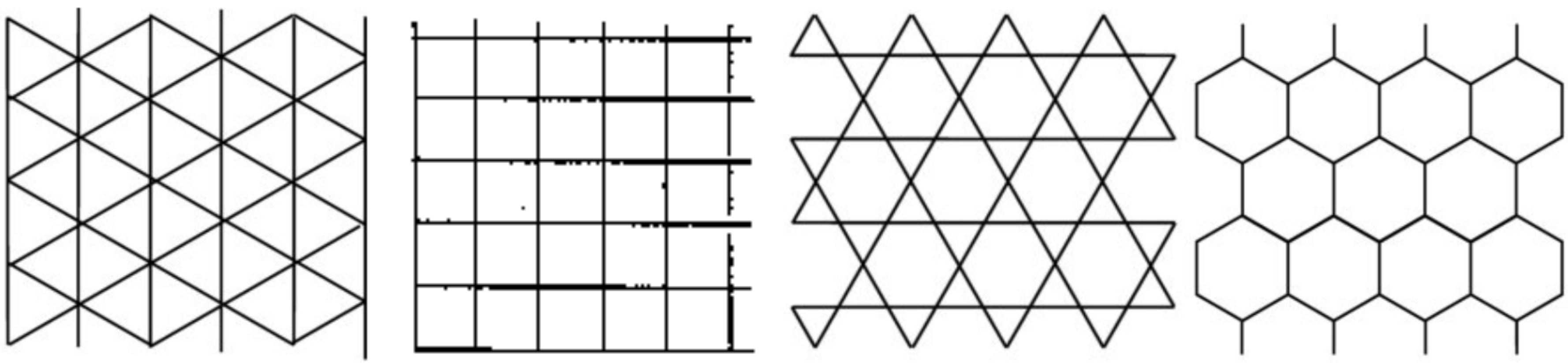
Configurazione dopo un riarrangiamento casuale dei legami

Diffusione H: Creazione/distruzione canali di conduttività





Percolation on different lattices



TRIANGULAR	SQUARE	KAGOME'	HONEYCOMB
$z=6$	$z=4$	$z=4$	$z=3$
$p_c^{BOND}=0.3473$	$p_c^{BOND}=0.5000$	$p_c^{BOND}=0.45$	$p_c^{BOND}=0.6527$
$p_c^{SITE}=0.5000$	$p_c^{SITE}=0.593$	$p_c^{SITE}=0.6527$	$p_c^{SITE}=0.70$