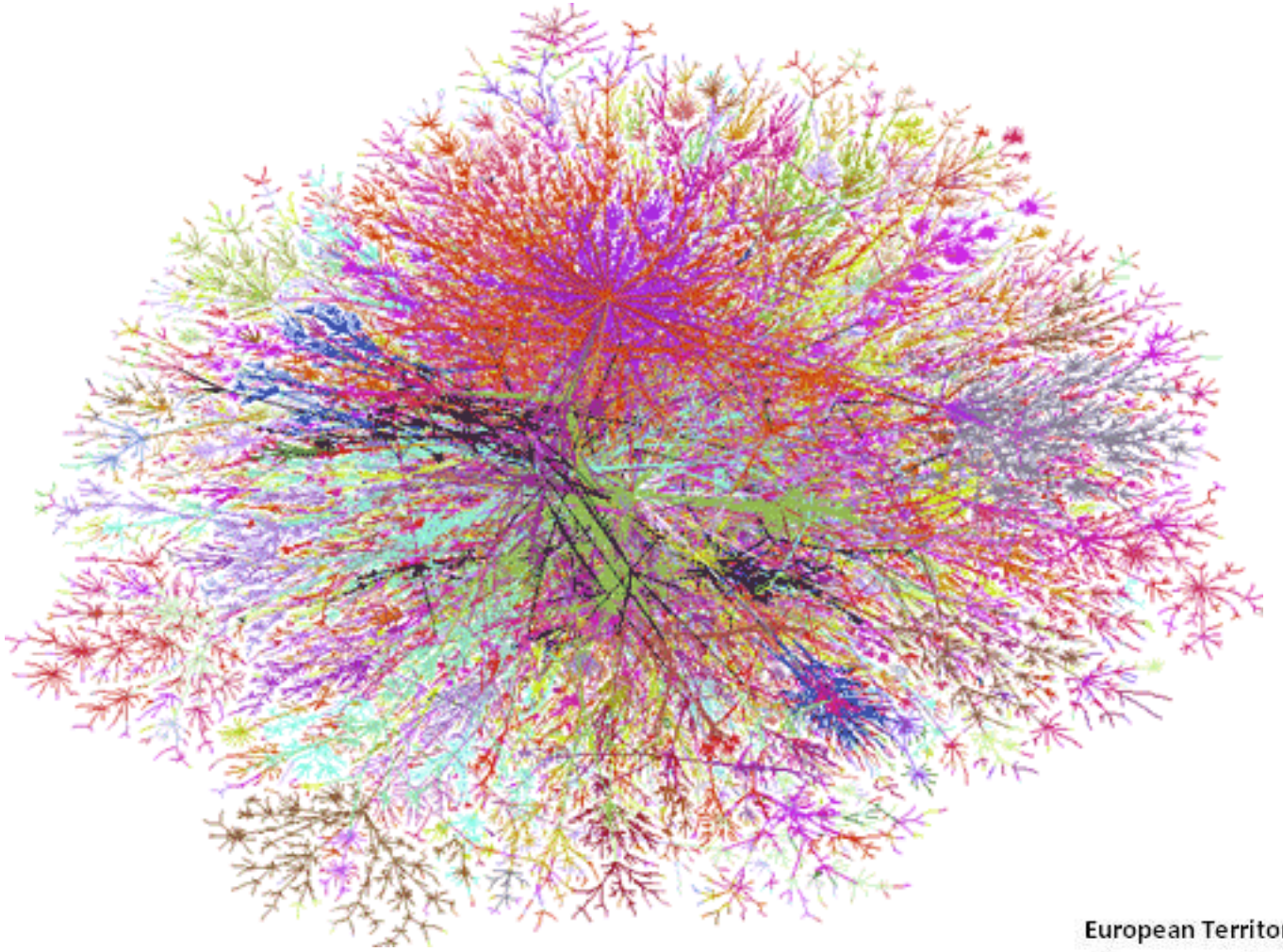
HELLENIC REPUBLIC
UNIVERSITY OF MACEDONIA
ECONOMIC & SOCIAL SCIENCES

ICoSCIS

Complex Science II



European Territorial Cooperation Programme
Greece-Bulgaria 2007-2013
INVESTING IN OUR FUTURE

Blagoevgrad 2013

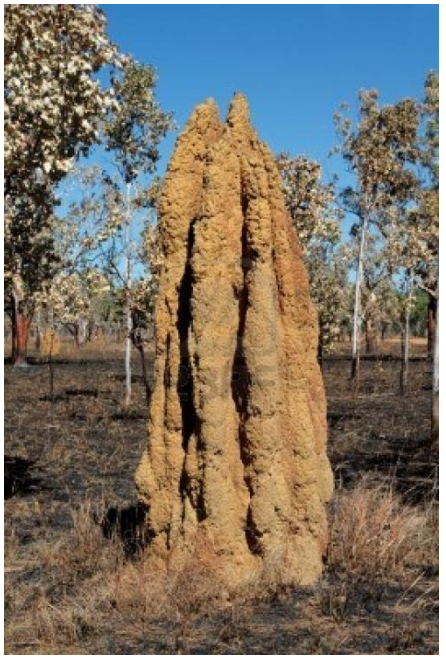
European Territorial Cooperation Progamme
Greece - Bulgaria 2007 - 2013

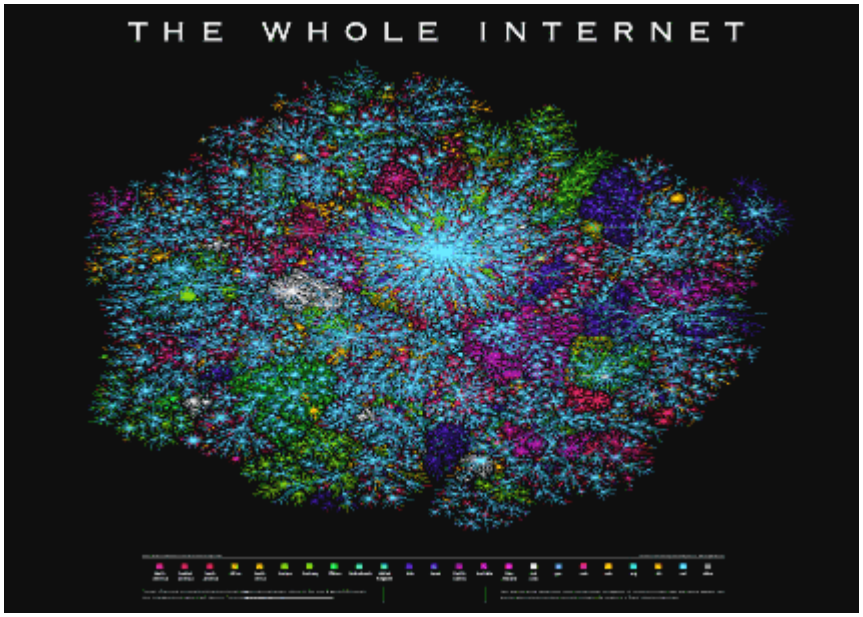
This Project is co-funded by the European Union (ERDF)
and National Funds of Greece and Bulgaria

What is a “complex system”

- Everyone is doing his job.
- There is NOT an architect.
- None of the parts knows the overall system.
- The system is self – assembled.

Examples..





Is Randomness something Complex?

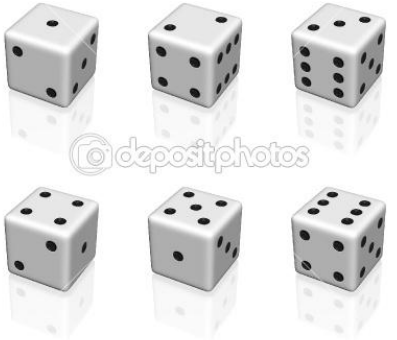
What is Random?

- Random = Something that we DO NOT decide!

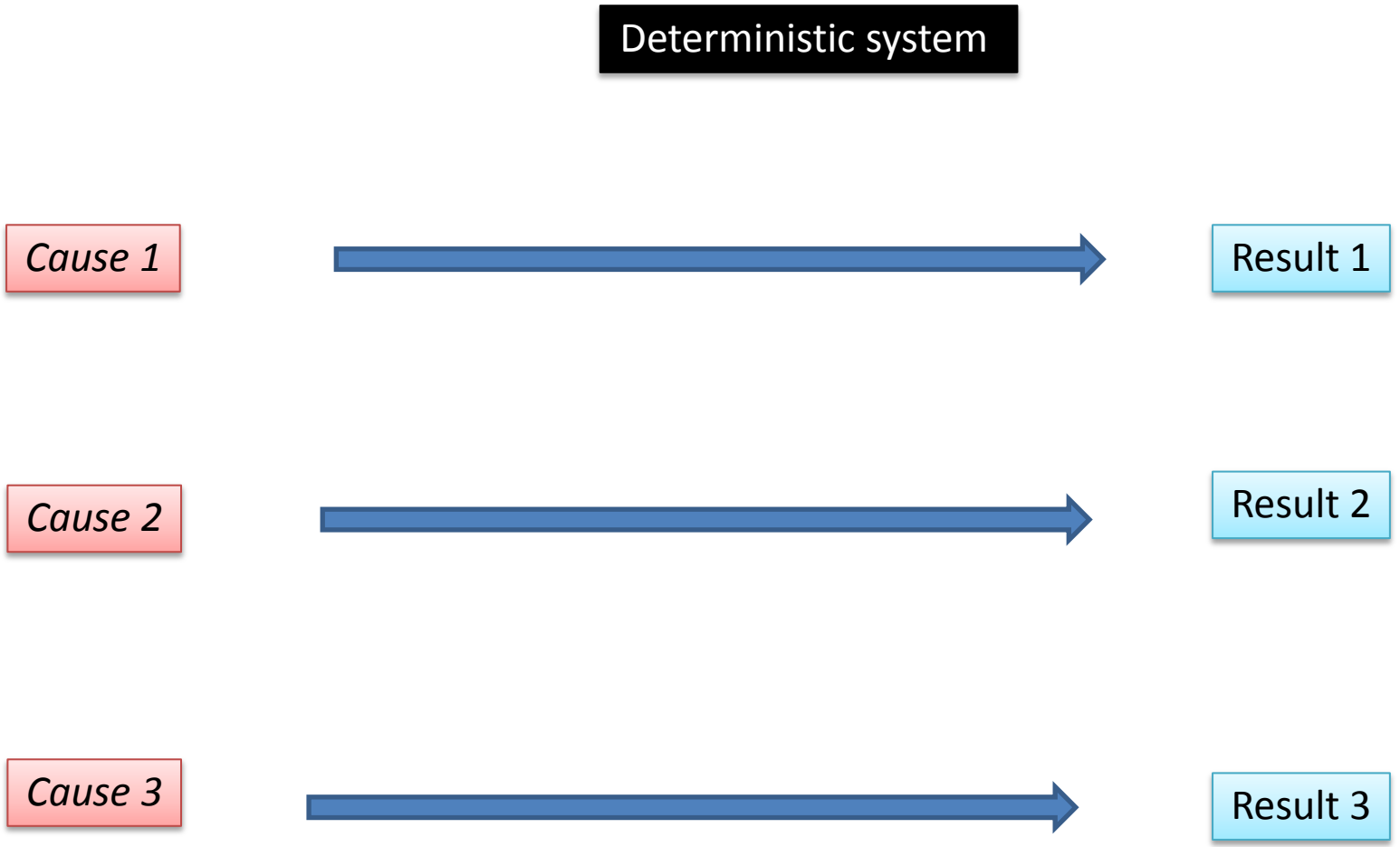
What exactly is Random ?

- If I drop a vase ⟹ the vase shall break.

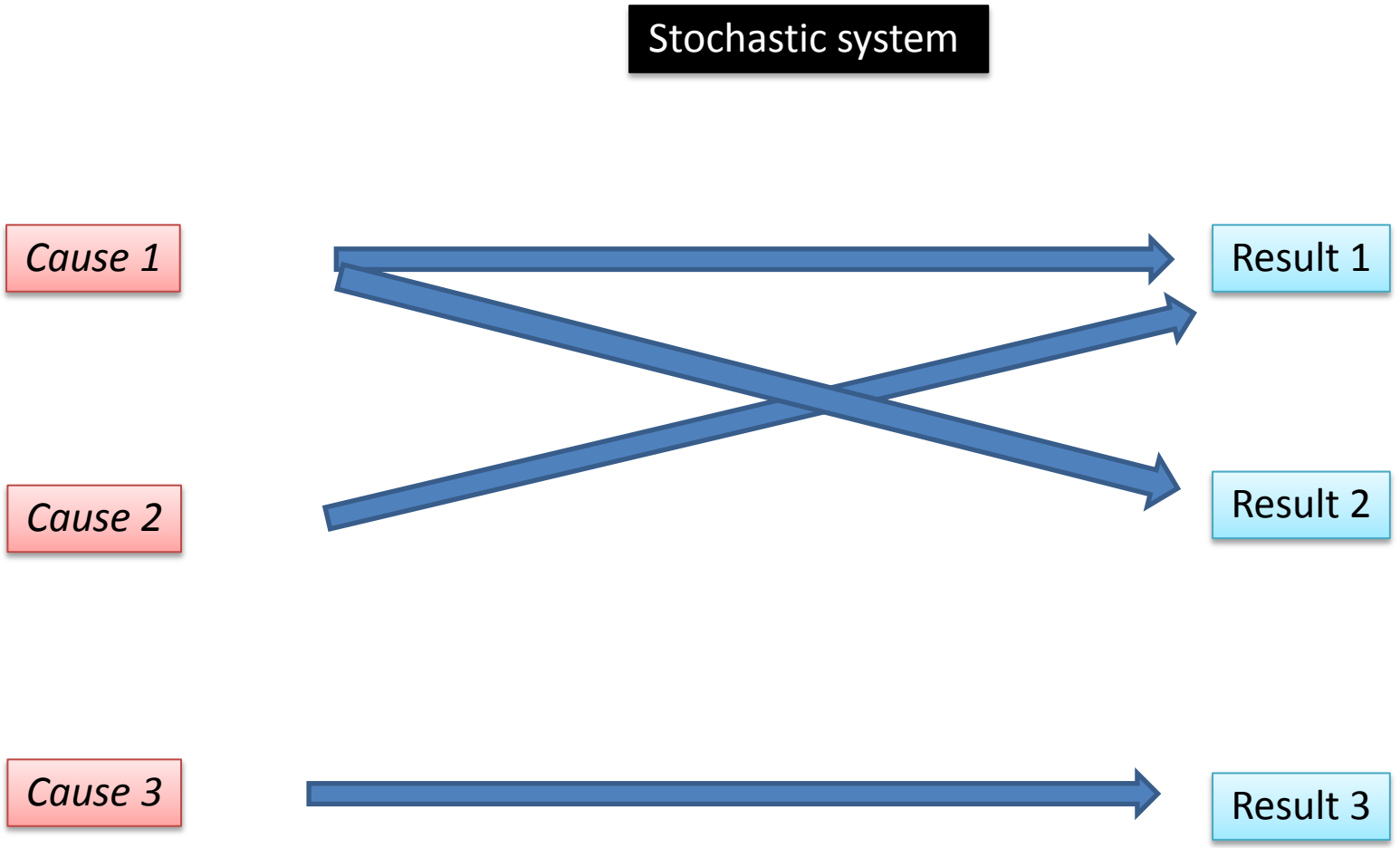
- If I roll a dice ⟹ the result will be 3.



Determinism vs *Stochastic*



Determinism vs *Stochastic*

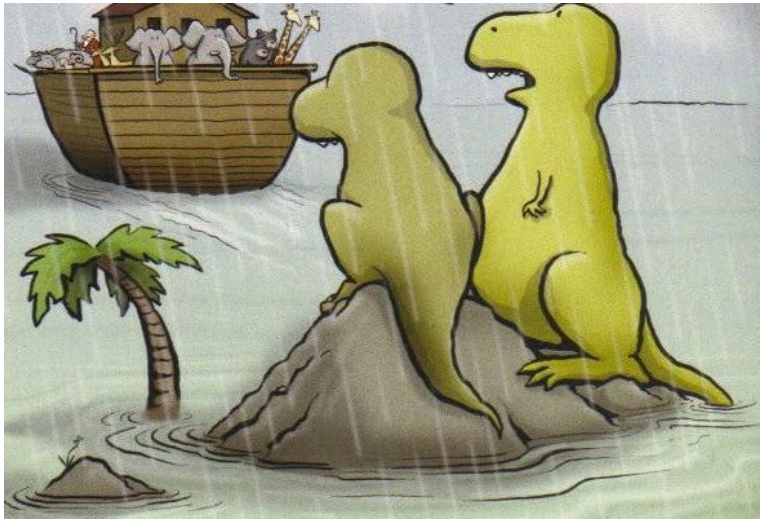


Randomness in our Every-day life

- Meet friends in the street..
- Catch the Bus..
- Walk around in the markets..
- Winning the lottery..

Randomness in Nature

- Will it rain tomorrow?
- Will I get sick this year?
- How different species appear or/and extinct?
- When will be the end of the human race?



Random Numbers

- A random number plays the role of the independent variable x of a given function y = f(x).

Let, $f(x) = \alpha x^2 / (5x - \beta x^5)$

Where x ϵ [0,1]

So, x can be any number in the ratio [0,1] and nobody knows which one!

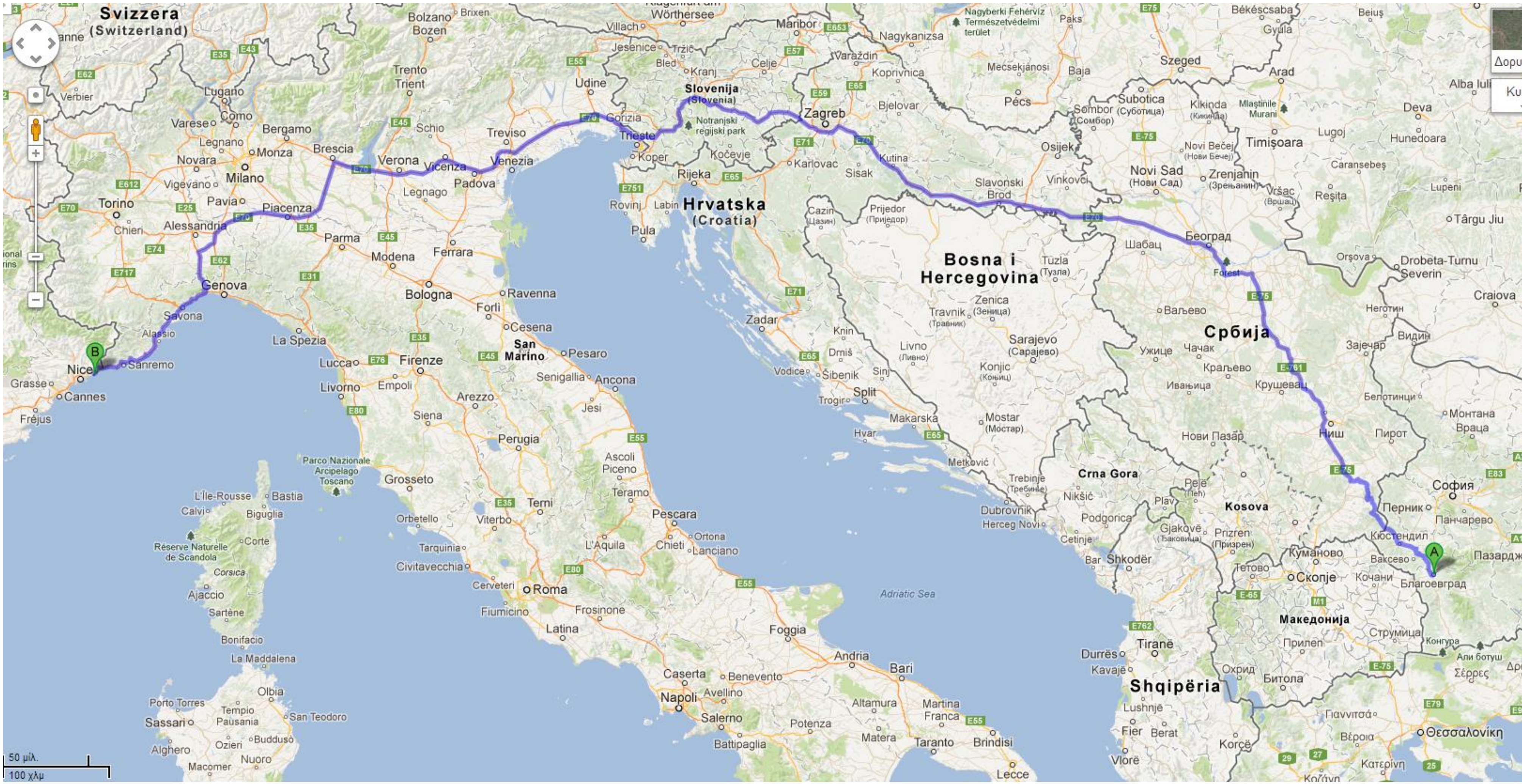
Modeling with Random Numbers

- An example..

Hit as many dishes as you can!!

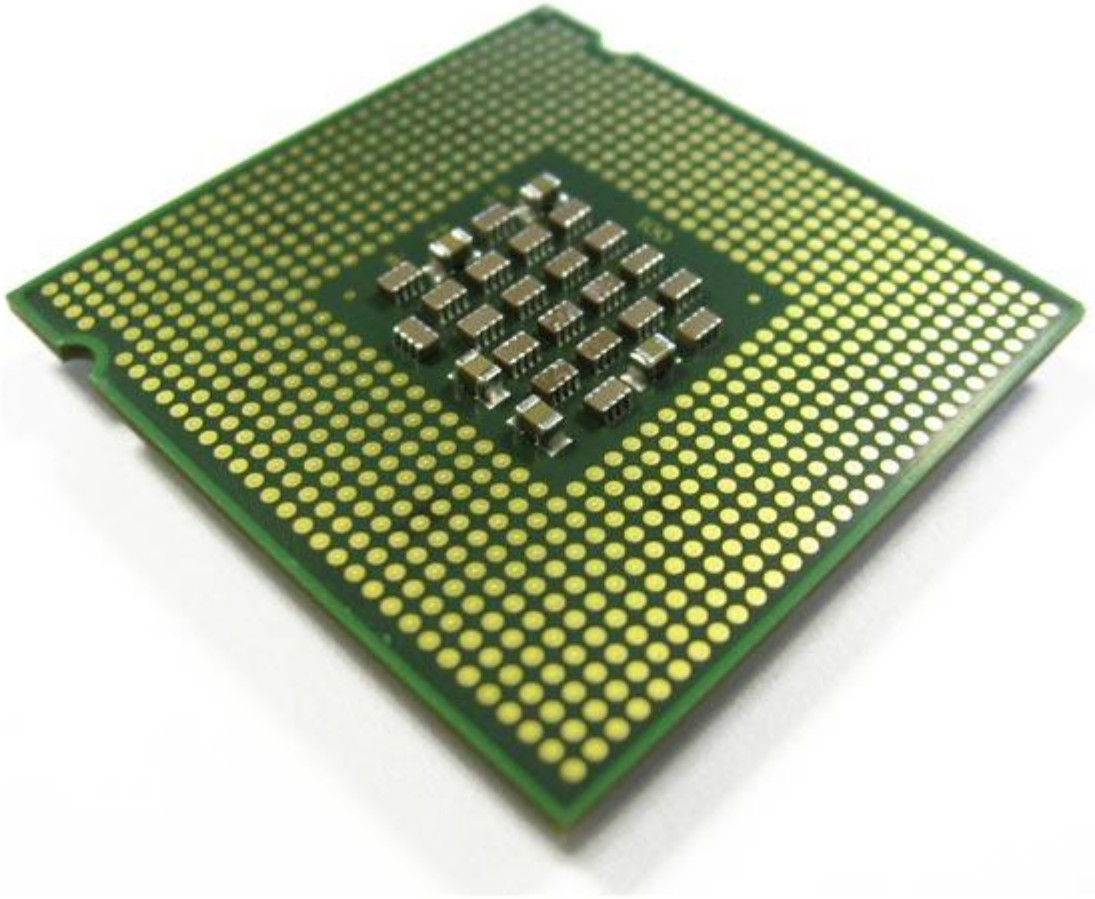
Where can I find a random Number?

CASINO Monte-Carlo



Duration of the trip to Monte-Carlo : ***aprox. 17 hours !***

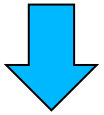
.. Ok this is quite far!
Somewhere else?



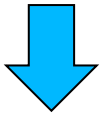
CPU - Central Processing Unit

Modeling with Random Numbers

CPU



Random number Generator



Random number

Independent variable of the problem.

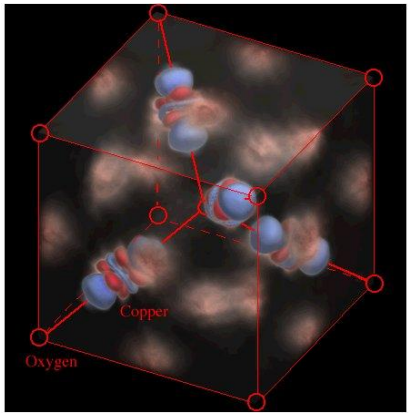
The truth is that we can NOT have absolutely random numbers!!

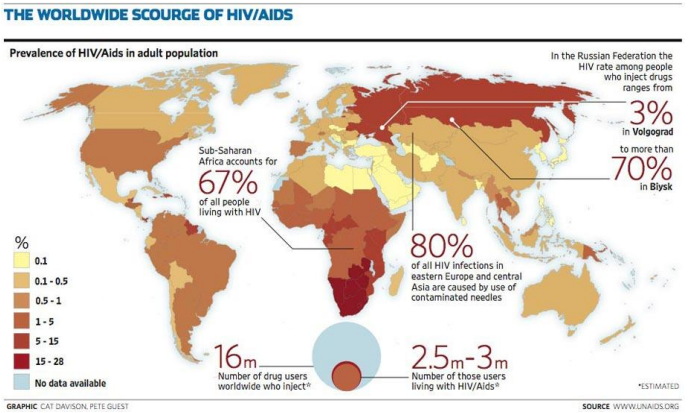
…But WHY modeling?

A simulation is a procedure that takes place virtually in a machine.

Even because the ***timeframe / space*** of the experiment is to small or large! NOT in human observable size!

Even because the experiment has ***not*** a human observable parameters.





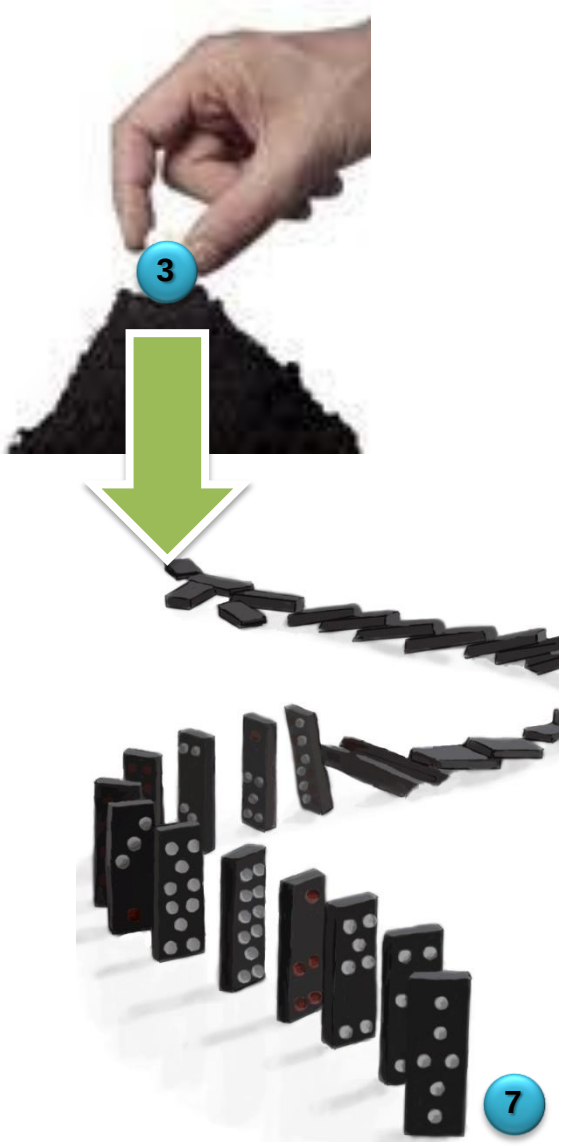
Modeling with Random Numbers

“FAKE” random numbers.

Quasi-Random numbers.

The Seed is the generation point of all numbers.

Quasi-Random numbers.



RANDOMNESS

C++

7 → 34 → 54 → x = rand();

Modeling with Random Numbers

- X = random number
- X = value of all possible ones depending the problem we want to study.
- We can NOT decide about the value of X.
- We solve the function Y = f(X).
- Y can be a number, event, state, another variable, etc.

Modeling with Random Numbers

Monte Carlo Simulation

- A simulation based on random numbers.
- Each independent simulation is been repeated many times.
- We extract the mean value of the wanted parameters.

Modeling with Random Numbers

50 %

50 %

16.66 %

Monte Carlo Simulation

- Let's find the mean value of 10 numbers which are between zero and one [0,1] .

X1=0.25
X2=0.02
X3=0.58
X4=0.64
X5=0.33

X6=0.78
X7=0.05
X8=0.10
X9=0.41
X10=0.59

Mean value <X> = 0.375

Monte Carlo Simulation

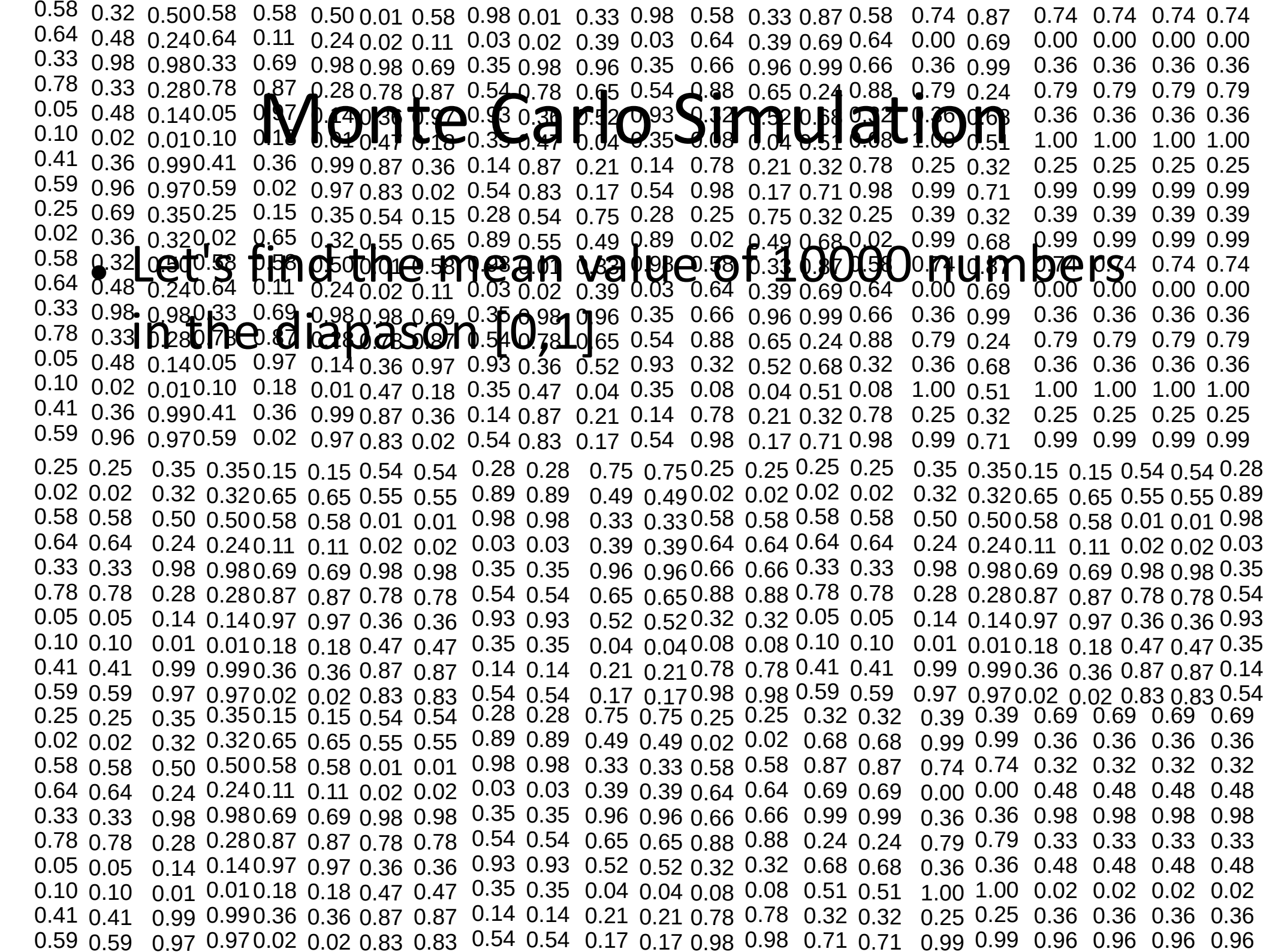
- Let's find the mean value of 100 numbers in the range between [0,1]

0.25	0.35	0.15	0.54	0.28	0.75	0.25	0.32	0.39	0.69
0.02	0.32	0.65	0.55	0.89	0.49	0.02	0.68	0.99	0.36
0.58	0.50	0.58	0.01	0.98	0.33	0.58	0.87	0.74	0.32
0.64	0.24	0.11	0.02	0.03	0.39	0.64	0.69	0.00	0.48
0.33	0.98	0.69	0.98	0.35	0.96	0.66	0.99	0.36	0.98
0.78	0.28	0.87	0.78	0.54	0.65	0.88	0.24	0.79	0.33
0.05	0.14	0.97	0.36	0.93	0.52	0.32	0.68	0.36	0.48
0.10	0.01	0.18	0.47	0.35	0.04	0.08	0.51	1.00	0.02
0.41	0.99	0.36	0.87	0.14	0.21	0.78	0.32	0.25	0.36
0.59	0.97	0.02	0.83	0.54	0.17	0.98	0.71	0.99	0.96

Mean value <X> = 0.445

Monte Carlo Simulation

- Let's find the mean value of 10000 numbers in the range between [0,1]

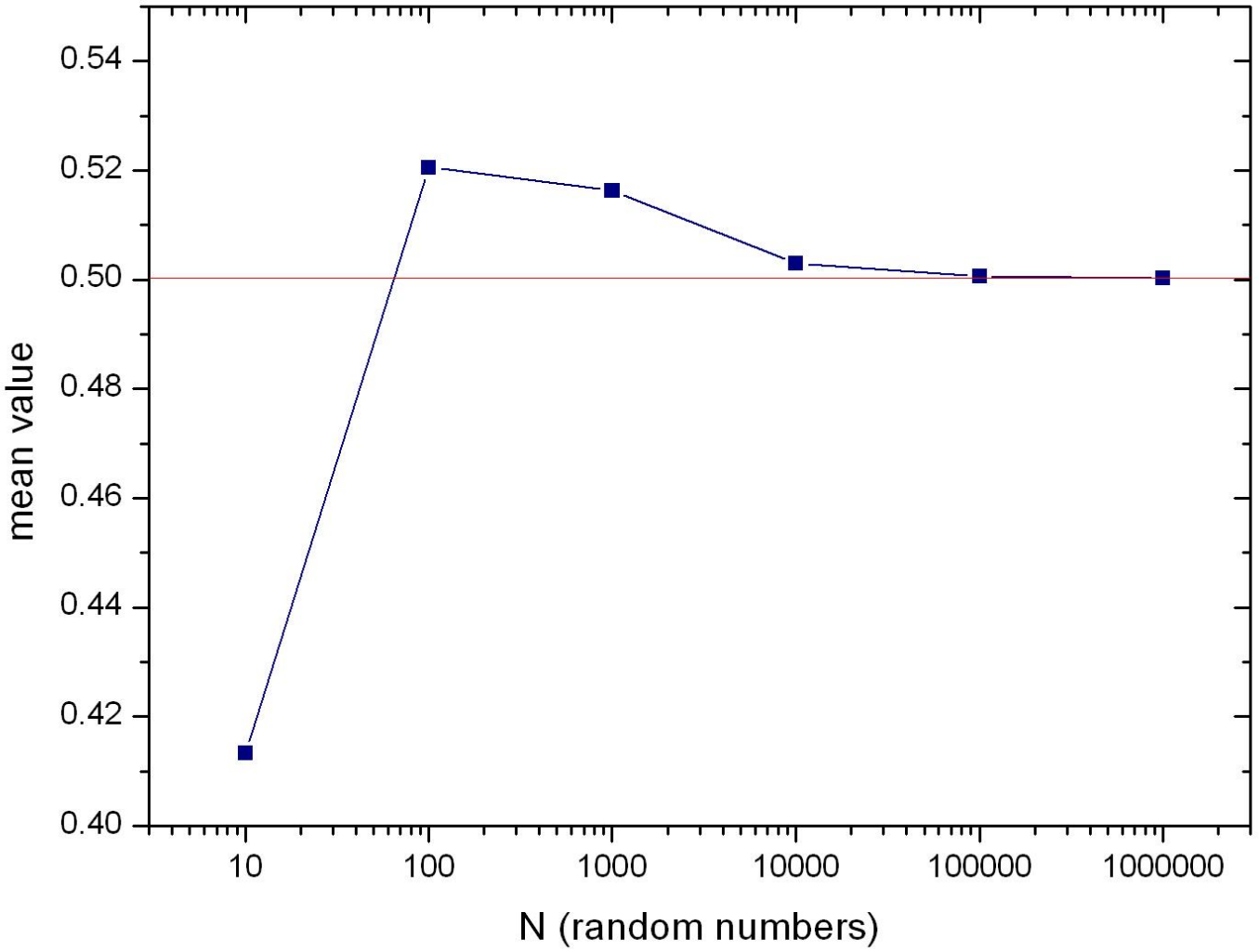

Monte Carlo Simulation
• Let's find the mean value of 10000 numbers in the diapason [0,1]

Monte Carlo Simulation

- Let's find the mean value of 10000 numbers in the range between [0,1]

Mean value <X> = 0.51

Monte Carlo Simulation



Monte Carlo Simulation

Example: Find the mean value of N random numbers between [0,1].

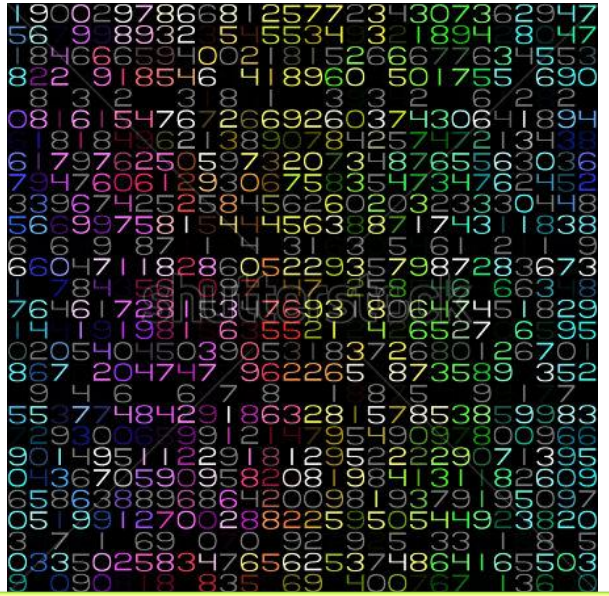
```
int ran_num,N=1000;
int seed=123456,i,sum=0;
double y,mean;
srand(seed);

   for(i=1;i<N;i++)
   {
        ran_num=rand();
        y=ran_num/(RAND_MAX);
        sum = sum + y;
   }

mean=sum/N;

printf("\t\t mean=%f\n\n",mean);
```

y is the wanted number between [0 – 1]

The random number generator, generates numbers between [0 – 32767]

Monte Carlo Simulation

- Using our computers we can generate millions of random numbers just in few seconds!!
- The only thing we have to do is to "command" the computer to calculate the mean value of all.
- We are finally too close to the arithmetical value of
- <X> = 0.5000



Monte Carlo Simulation

Example II : Find the mean value of 10^5 random numbers between [-100,+100].

tip..
You will need a transformation function

Monte Carlo Simulation

Example II : Find the mean value of 10^5 random numbers between [-100,+100].

tip..
You will need a transformation function

- Let y be the random number between [-100,+100]
- And let x be the random number in the range [0,1]
- The minimum value of x equals to zero
- for x = 0 : y = -100
- The maximum value of x equals to 1
- for x = 1 : y = +100
- y = 200x - 100

Monte Carlo Simulation

In general :

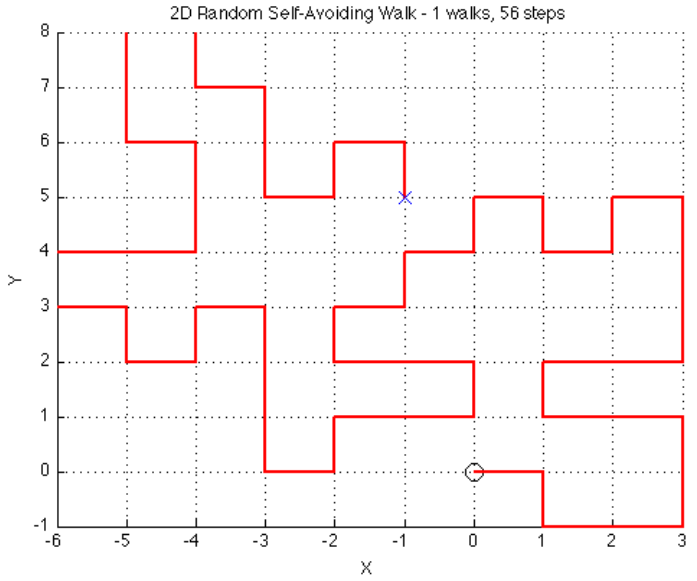
- Is a simulation using randomness as input.
- We repeat the same simulation many times.($>10^3$)
- The simulation has as an output the study parameter.
- We calculate the mean value of all 10^3 independent simulations.

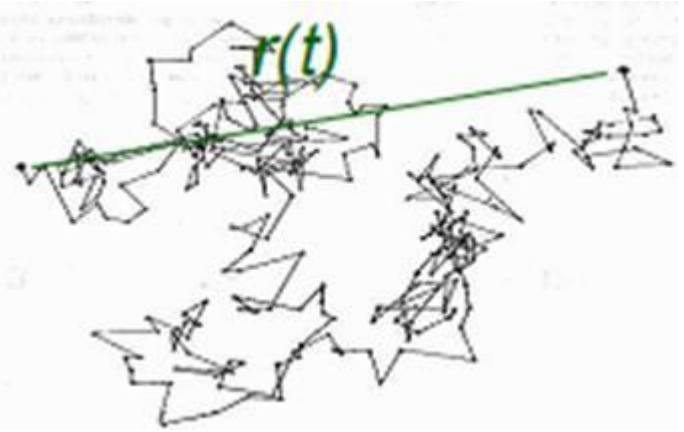
some homework …

- What is a complex system?
- What is a random number?
- How many random numbers can we have in a simple Monte-Carlo simulation?
- Can you create a random number generator which gives 1000 random numbers between [0,6]?
  - Can you create a program which calculates the mean value of all those 1000 numbers?

Random walk

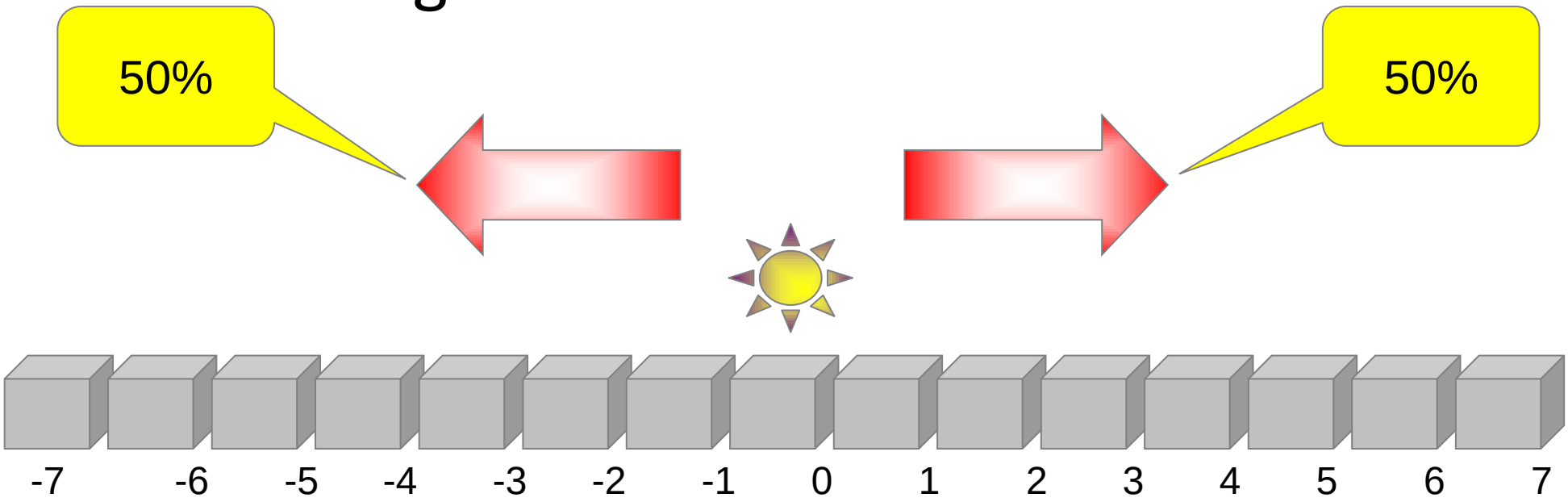
- Drunk man's walk
- Women go shopping
- Brown movement
- Electrons inside the solar cell
- Spreading of a disease
- … Your suggestion can be here..





Random Walk in a lattice

- Imagine an one-dimensional lattice
- Something like the movement of a train.



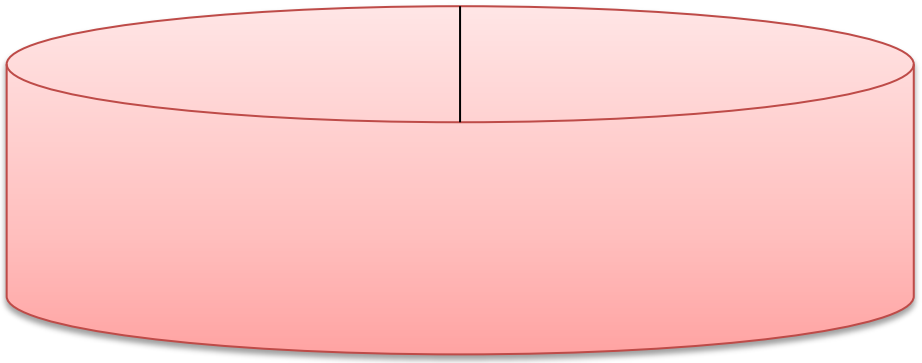
Random Walk in a lattice

- 1D lattice:

A dice with only two different possible events

How to simulate this kind of dice?

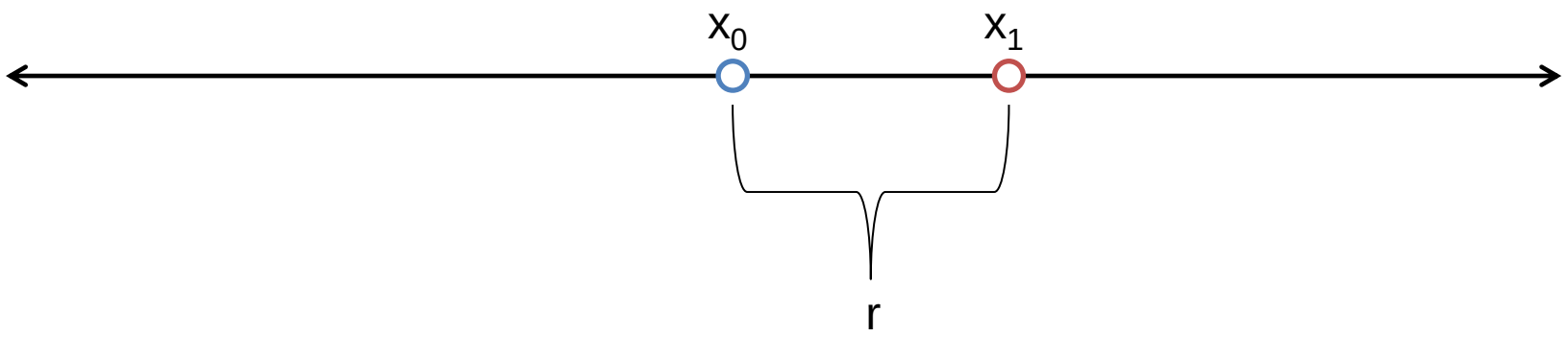
Basic Idea:



Computer Analog:

Random Walk in a lattice

$$\Delta x = x_1 - x_0$$



x_0 = the initial site of the random walker.

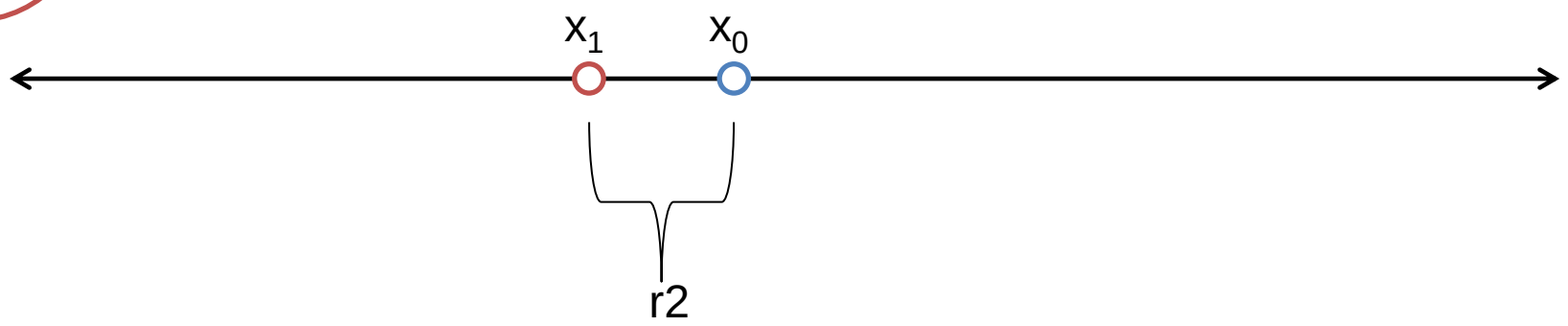
x_1 = the final site of the random walker.

Δx = the displacement.

Random Walk in a lattice

2

$$\Delta x = x_1 - x_0$$



x_0 = the initial site of the random walker.

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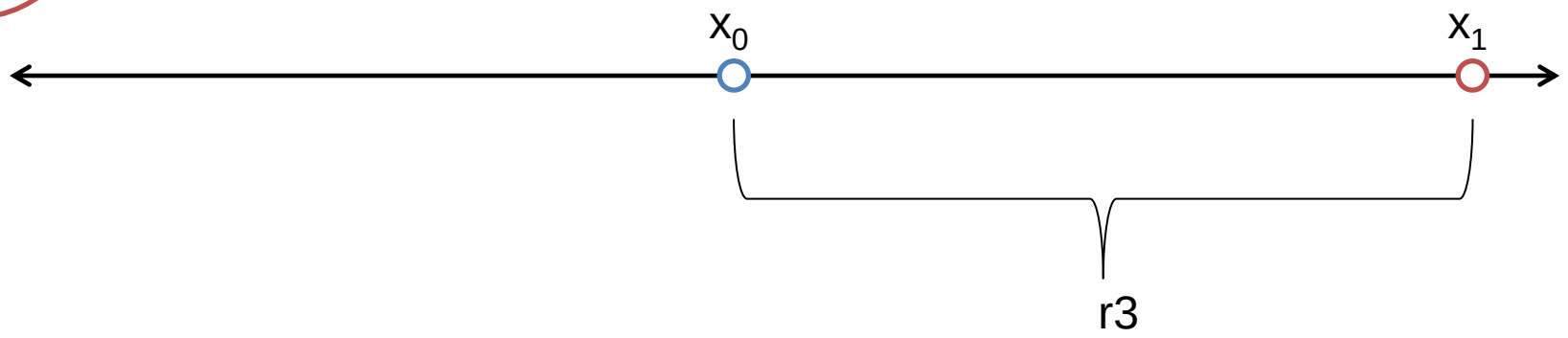
Random Walk in a lattice

3

$$\Delta x = x_1 - x_0$$



x_0 = the initial site of the random walker.

x_1 = the final site of the random walker.

Δx = the displacement.

Random Walk in a lattice

- *After N simulations we can calculate the mean value of all Δx.*
- *Let $x_0 = 0$*

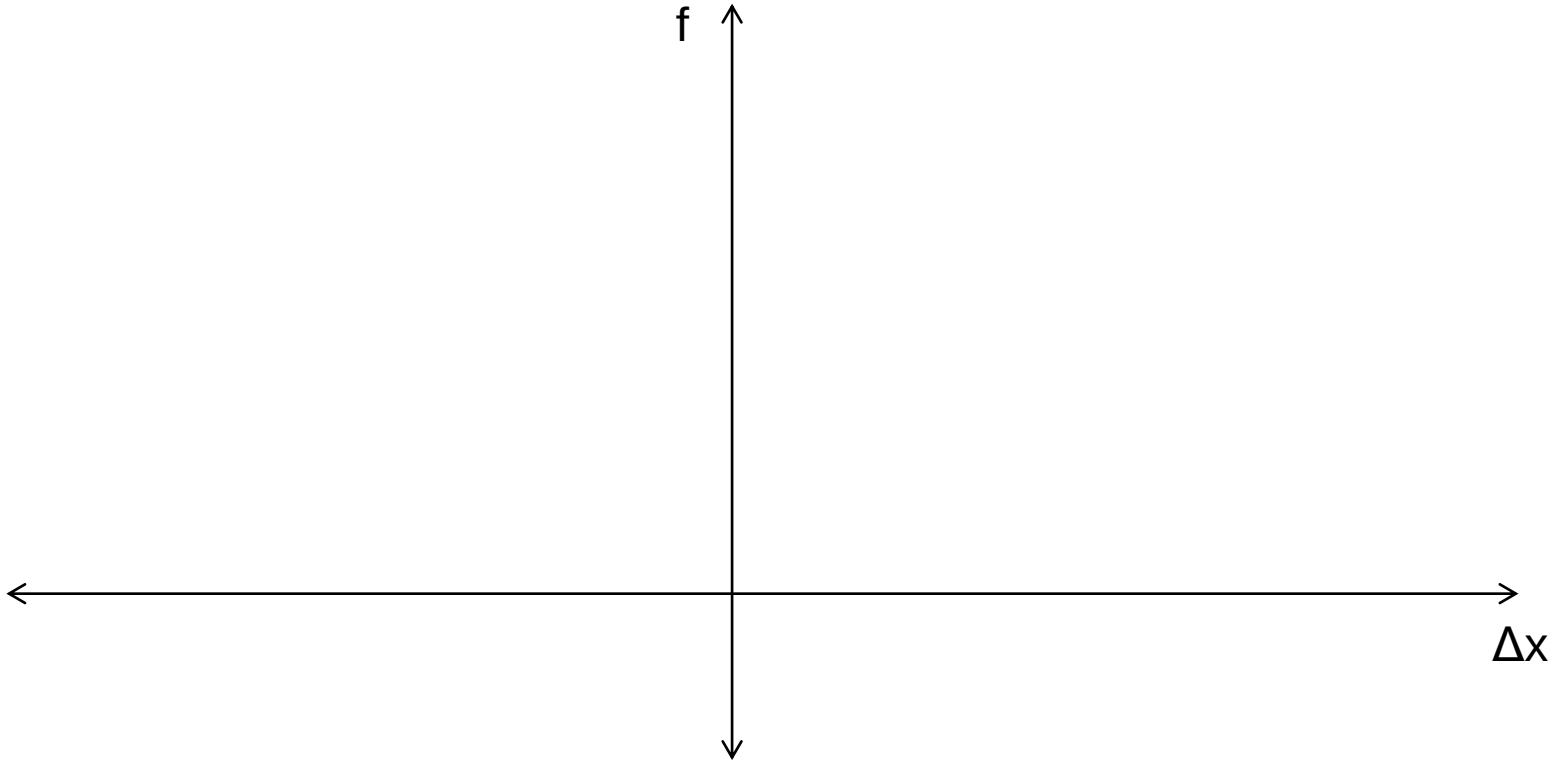
Simulation	Δx
1	5
2	-2
3	8
4	0
5	3
6	-1
7	0
8	-2
9	1
…	…
N	3

$$\langle \Delta x \rangle = (x_1 + x_2 + x_3 + \ldots + x_N) / N$$

Random Walk in a lattice

Can you imagine the mean value of Δx ?

The distribution of all Δx



Random Walk in a lattice

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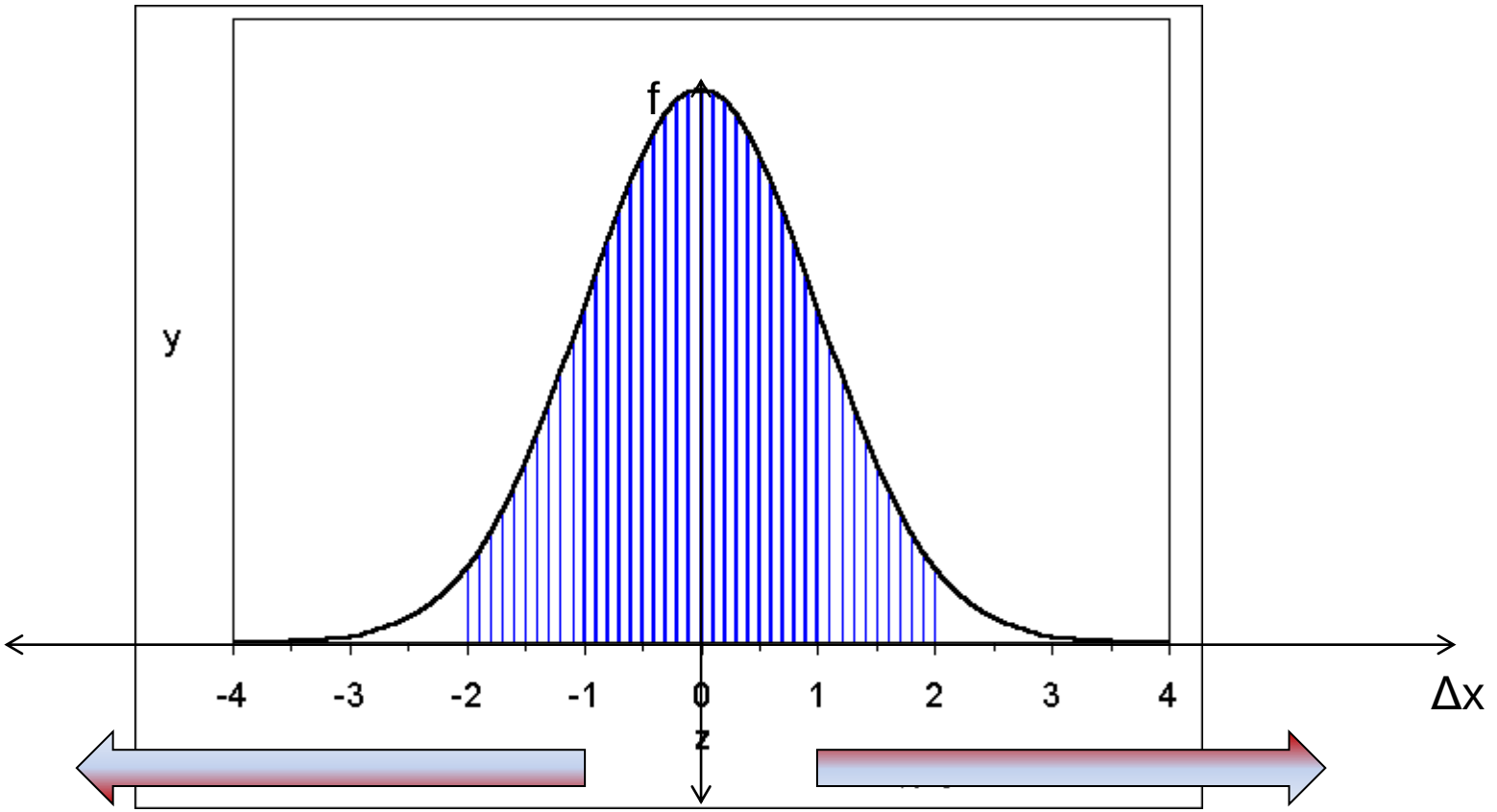
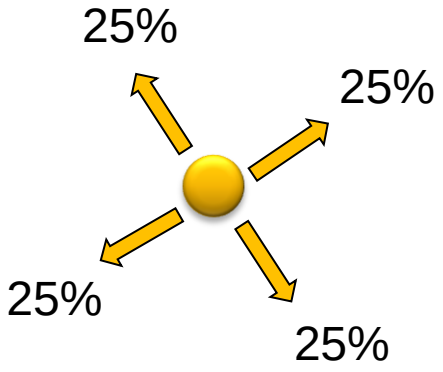
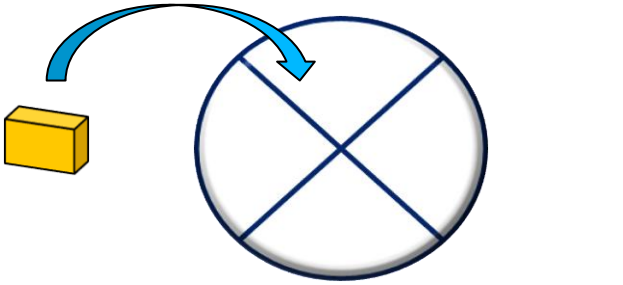
The distribution of all Δx

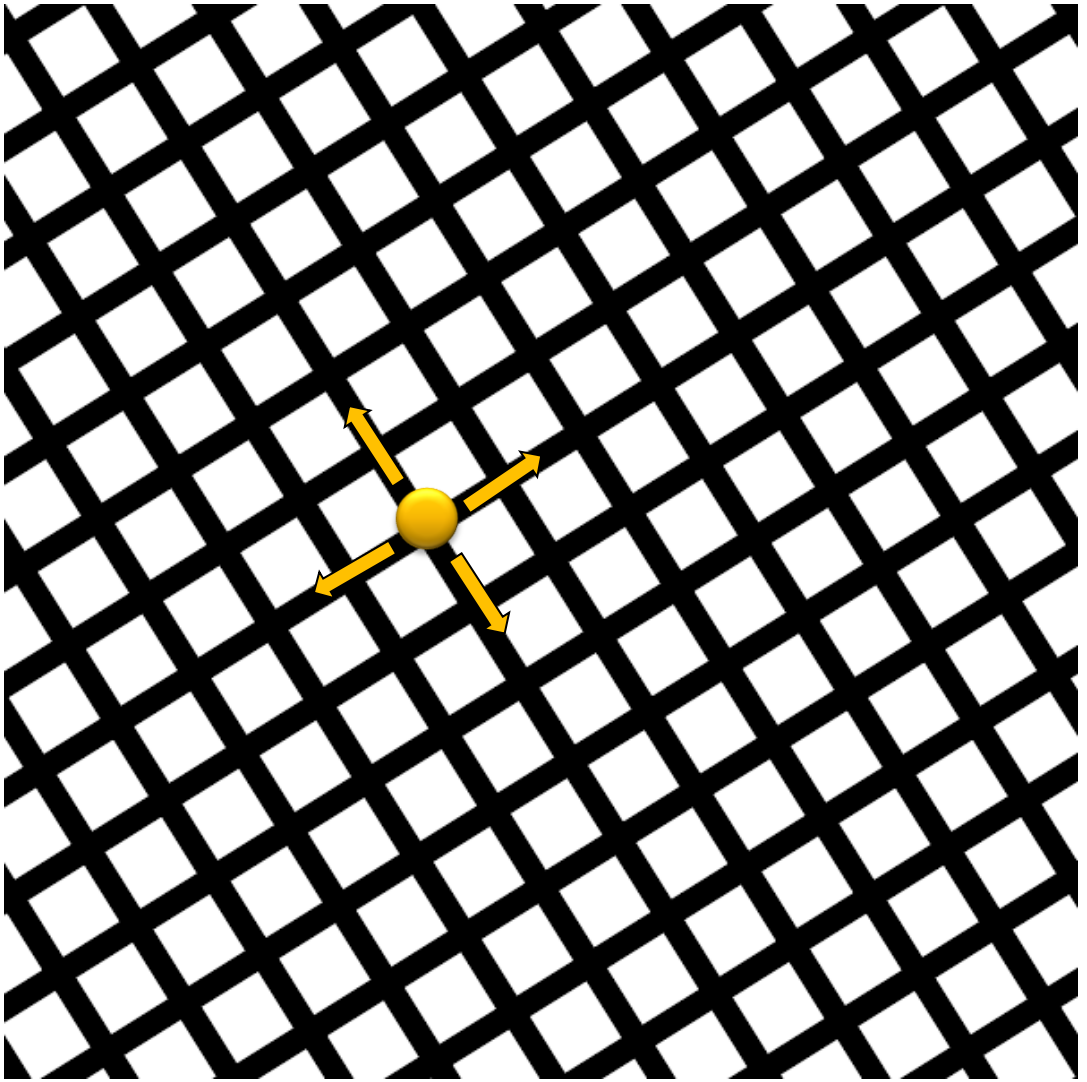


Random Walk in a lattice

- 2D lattice



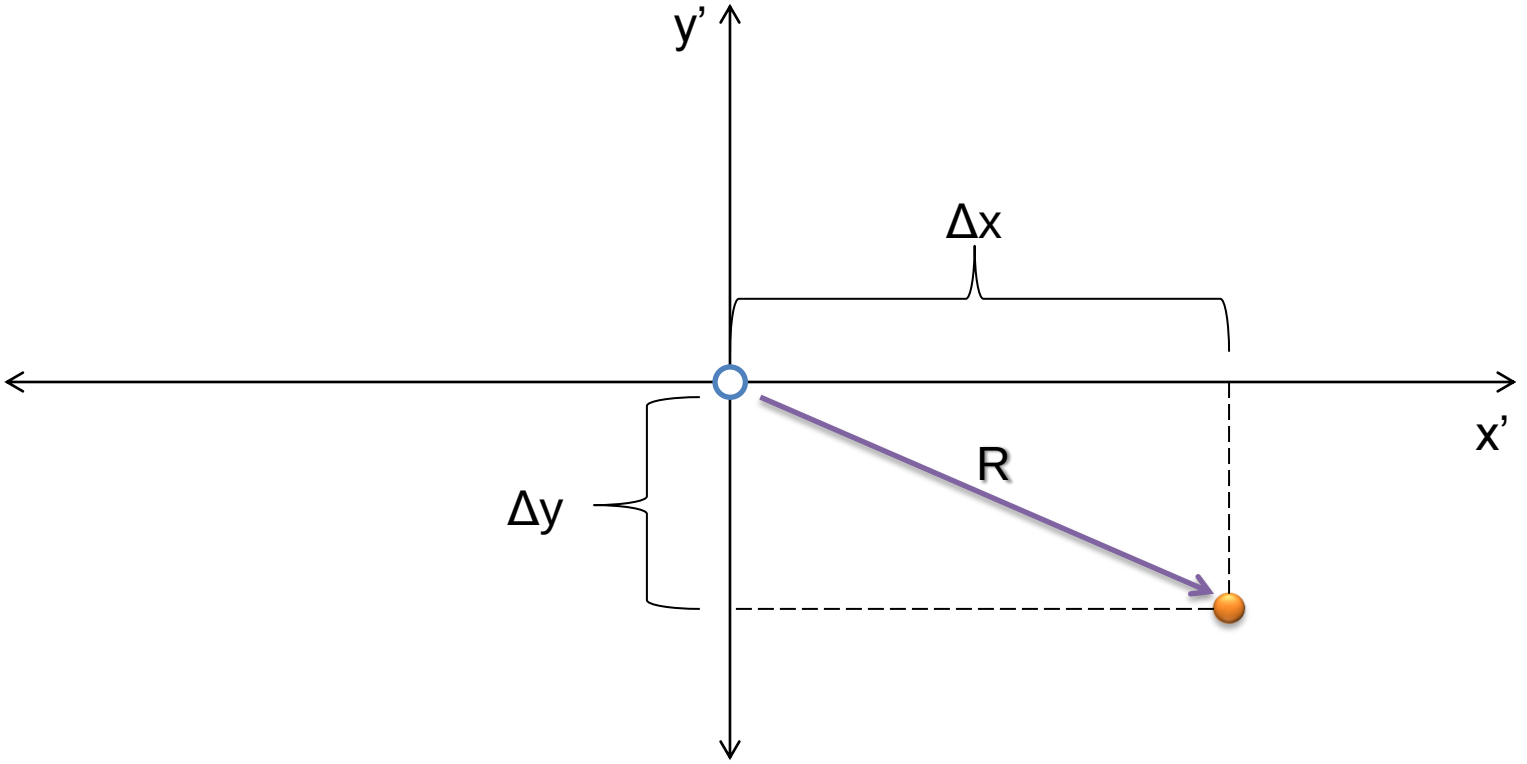




Random Walk in a lattice

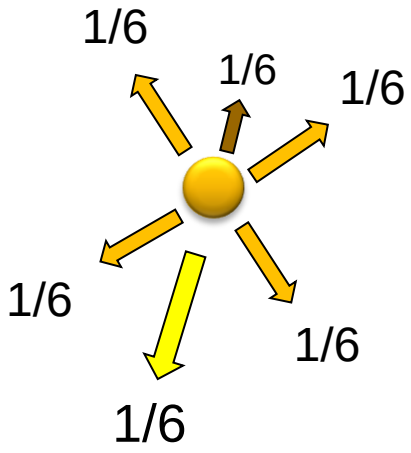
The square displacement :

$$R^2 = (\Delta x)^2 + (\Delta y)^2$$



Random Walk in a lattice

- 3D lattice



Exercise 1

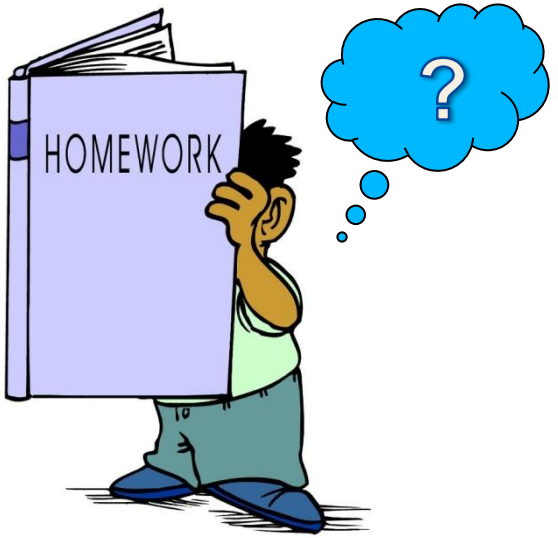
Random Walk

- *Create a program which performs a random walk for N = 1000 steps.*
- *You will do that for two cases:*

(a) an one dimensional system,

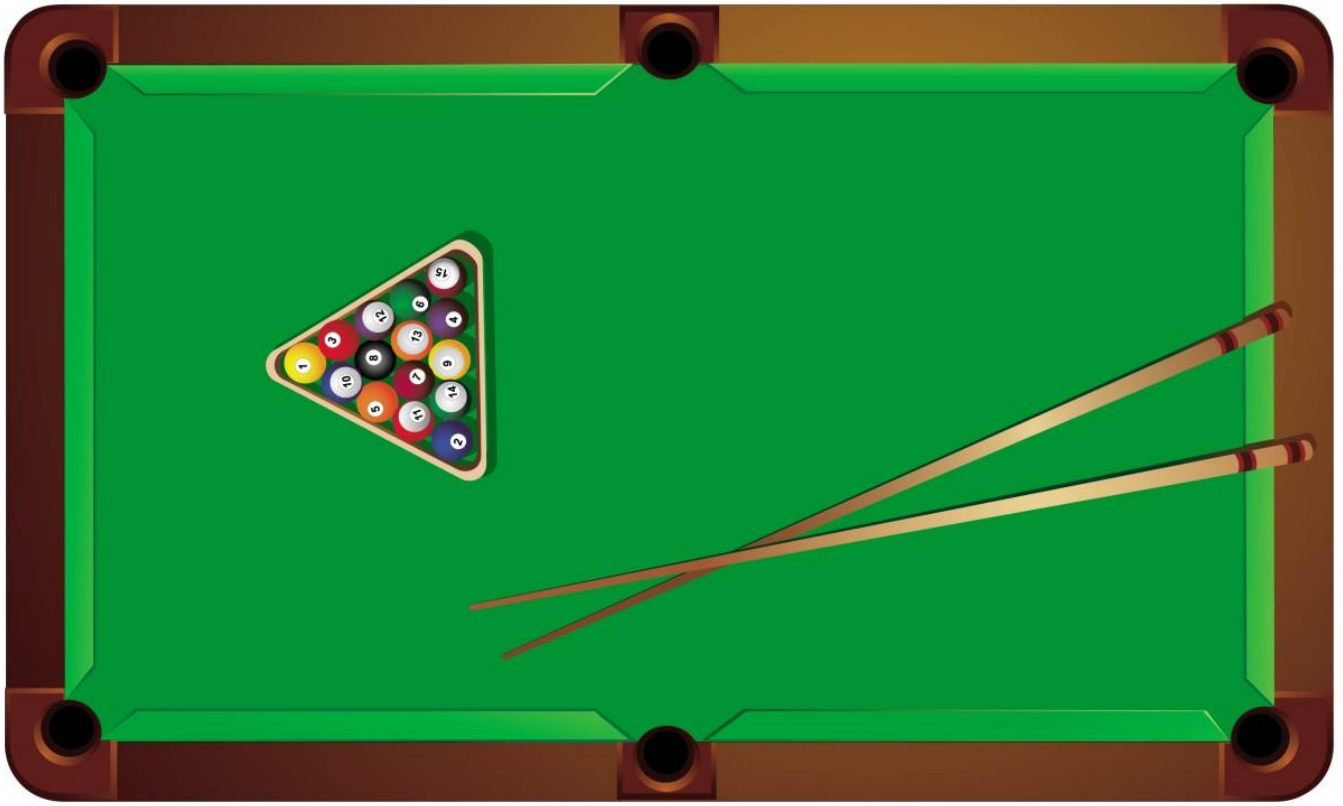
(b) a two dimensional system.

- *The program should calculate the square displacement R^2.*
- *Run the program for 10000 runs and find the mean square displacement, namely $\langle R^2 \rangle$.*



Let's take a break ..

The trapping problem

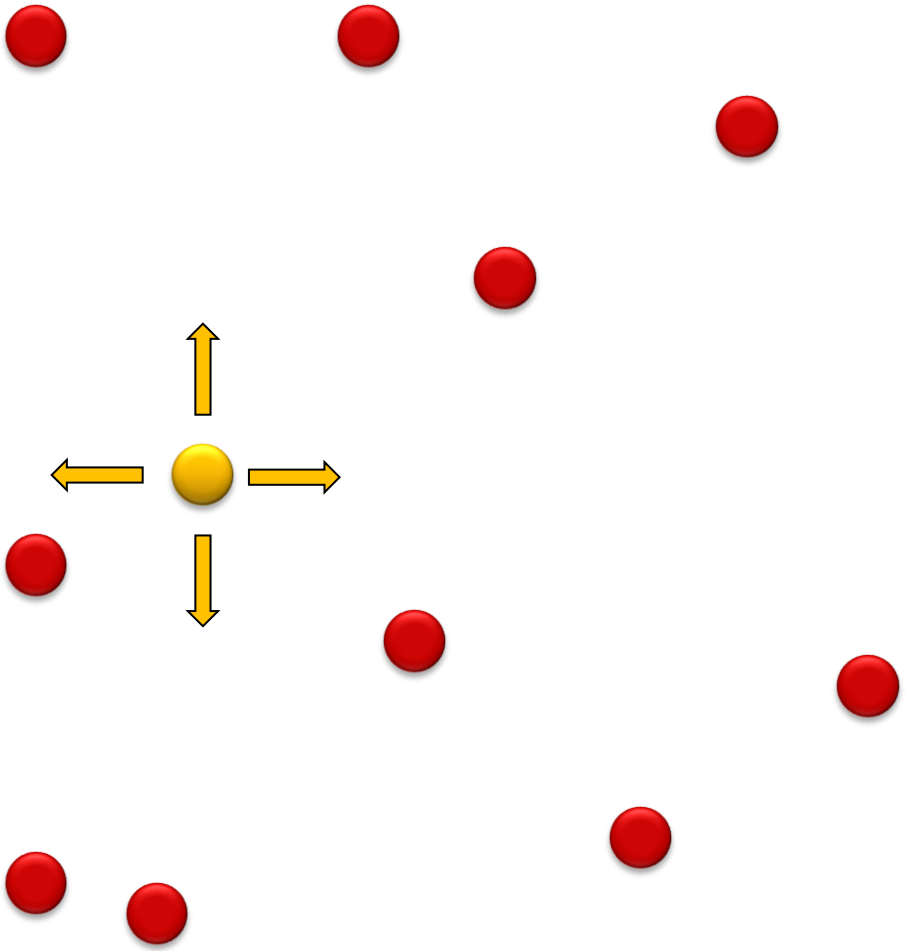


The trapping problem

Let's imagine that in the previous 2D system, we spread traps randomly in the lattice with a density c.

Example:
c = 10% means that for a lattice of 10x10 = 100 sites there are 10 traps randomly distributed in the system.

The traps maybe can represent an attractive potential – hole. etc..



The trapping problem

Is it possible for us to have a computer analog?

0	0	0	0	0	0	0	0	0	0	0	0
0	0	**1**	0	0	0	0	0	0	0	0	**1**
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	**1**	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0
0	0	**1**	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0
1	0	0	0	0	0	0	0	**1**	0	0	0
0	0	0	0	**1**	0	0	0	0	0	0	**1**
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	**1**	0	0	0	0
0	**1**	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	**1**	0
0	0	0	0	0	0	0	0	0	0	0	0

Trap

Empty site

The trapping problem

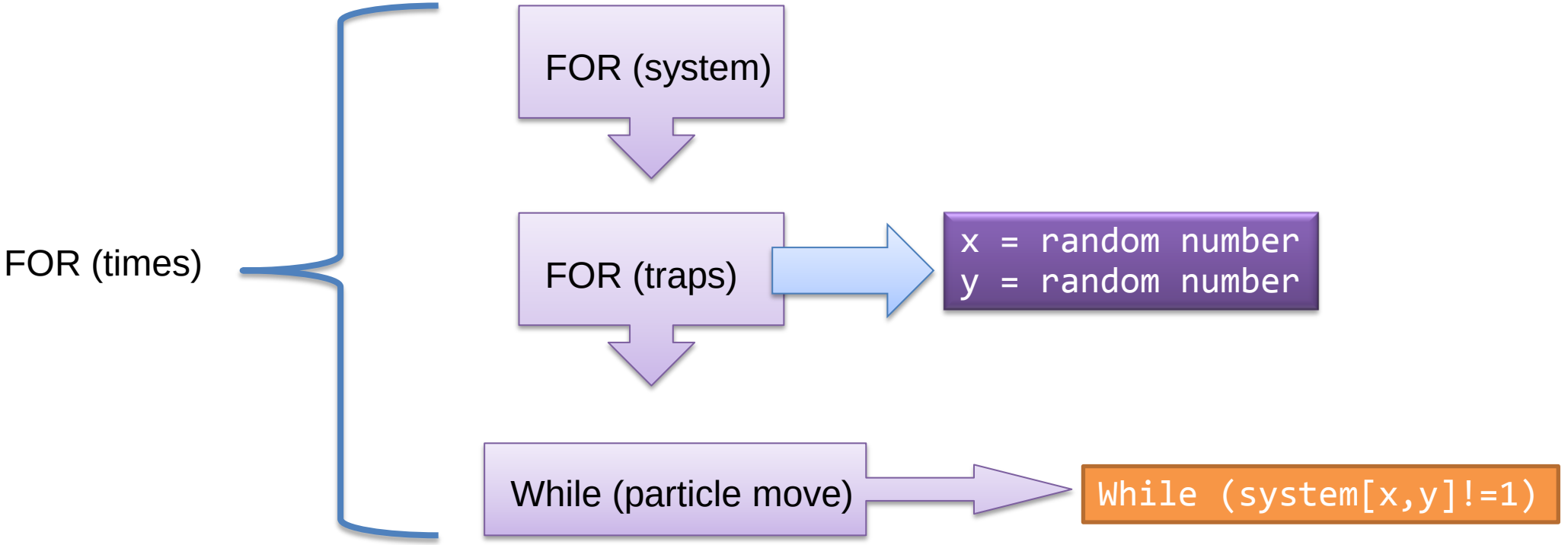
Particle	Trapping time
1	5
2	34
3	12
4	2
5	23
6	15
7	12
8	3
9	14
10	10
11	8
12	6
13	21
14	2
15	11
16	23
17	12
18	8
19	5
20	10
21	12
22	20

0	0	0	0	0	0	0	0	0	0	0	0
0	0	**1**	0	0	0	0	0	0	0	0	**1**
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	**1**	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0
0	0	**1**	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	**2**	0	0	0	0	0
1	0	0	0	0	0	0	0	**1**	0	0	0
0	0	0	0	**1**	0	0	0	0	0	0	**1**
0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	**1**	0	0	0	0
0	**1**	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	**1**	0
0	0	0	0	0	0	0	0	0	0	0	0

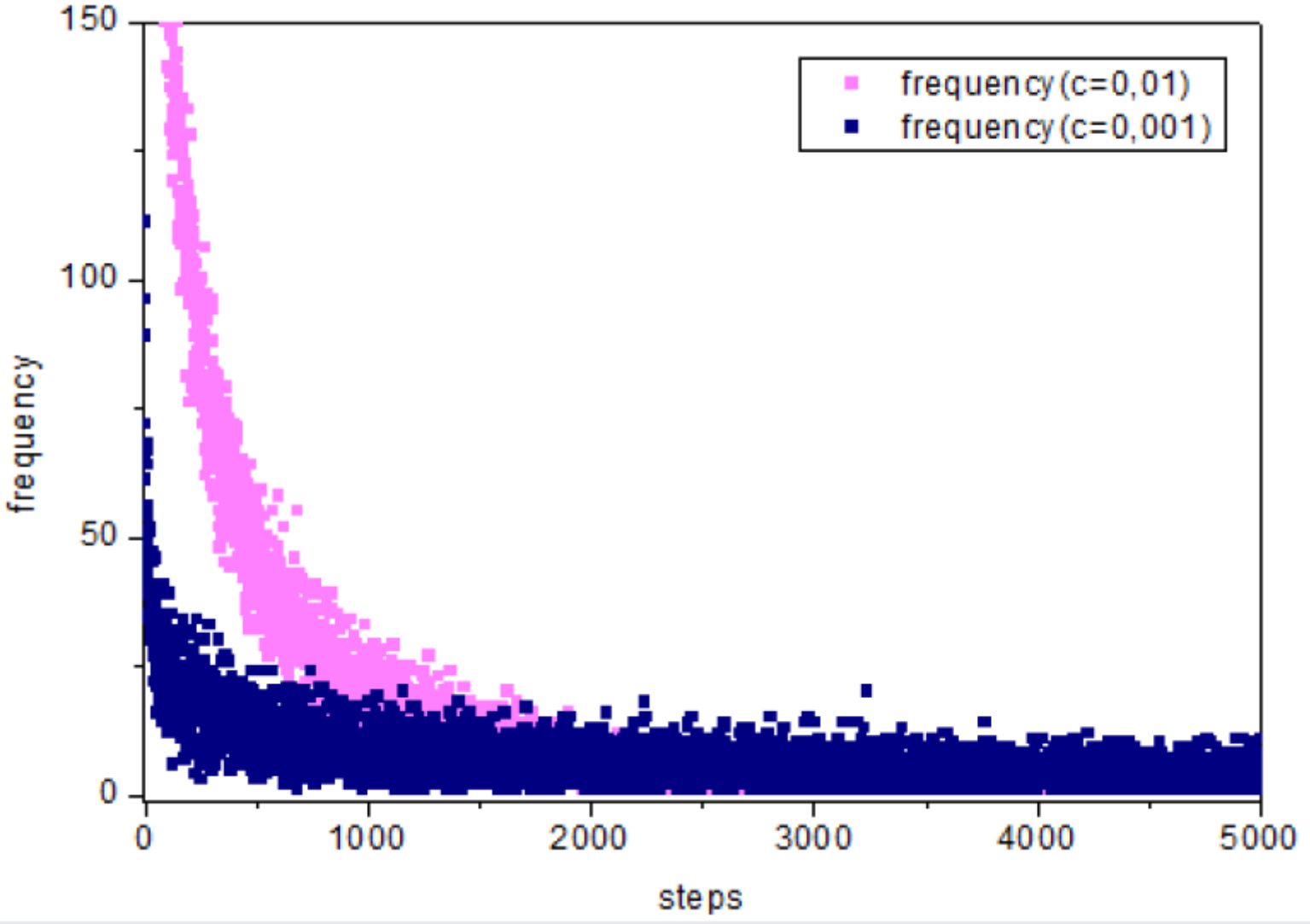
Trapping time	Frequency
1	0
2	1
3	1
4	0
5	2
6	1
7	0
8	2
9	0
10	2
11	1
12	4
13	0
14	1
15	1
16	0
17	0
18	0
19	0
20	1
21	1
…	…

The trapping problem

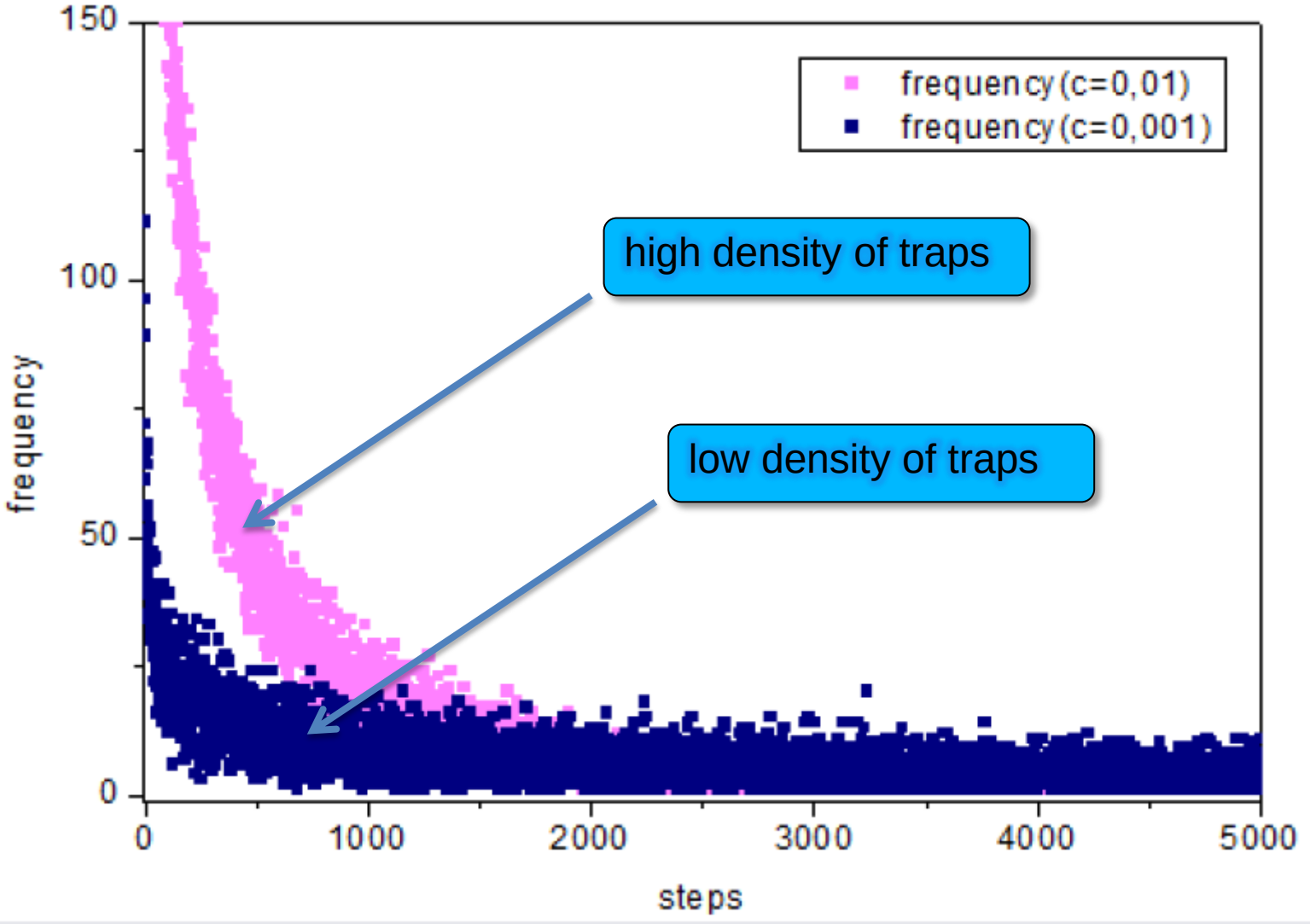
Example:
Create a program which generates a 2 dimensional lattice of size 100 x 100.
In this lattice place at random positions a number of trap molecules with concentration c.
Place one particle at a random position on the lattice and let it perform a random walk.
Perform this process for 100 times and find the mean trapping time.



The trapping problem

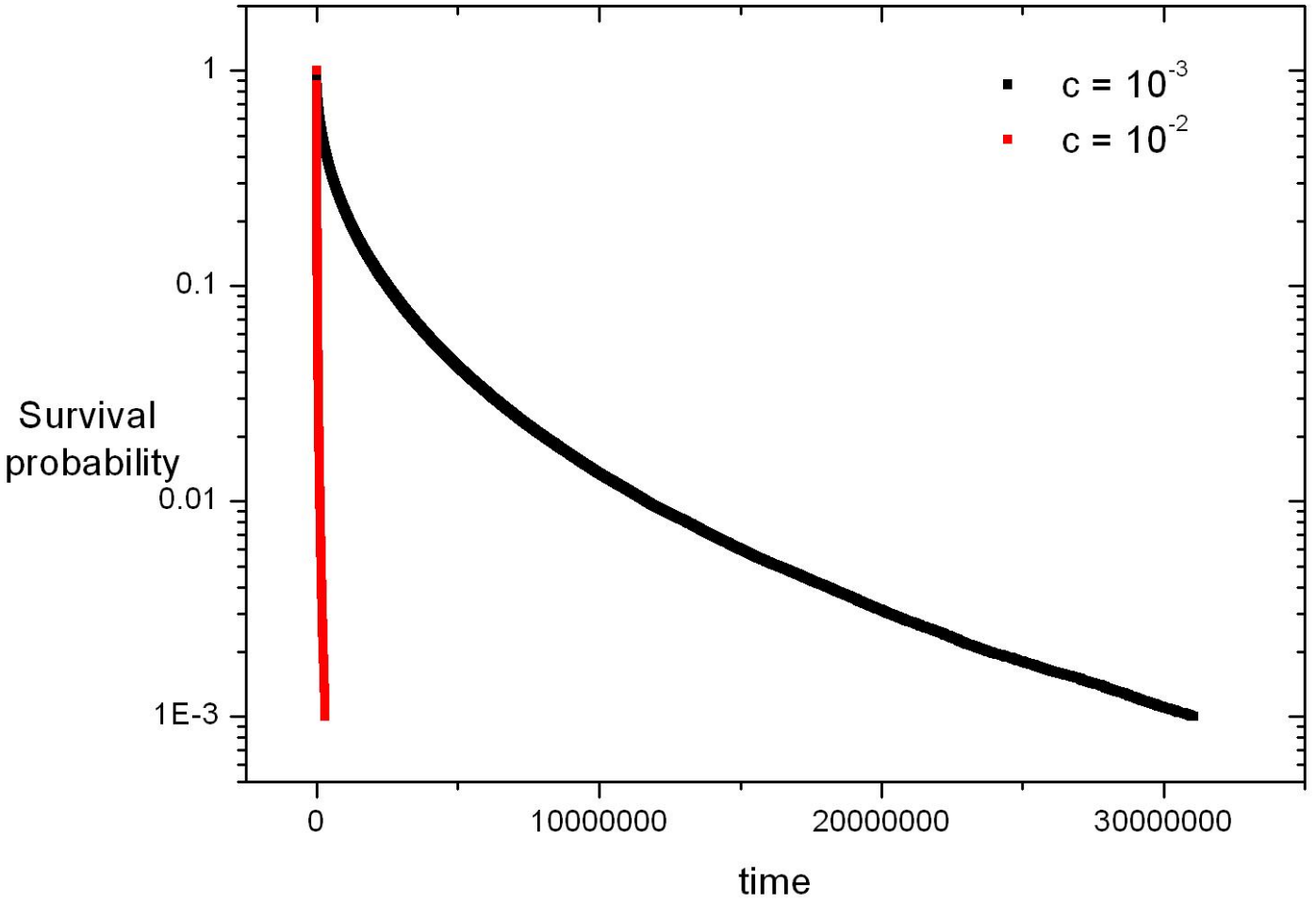


The trapping problem



The trapping problem

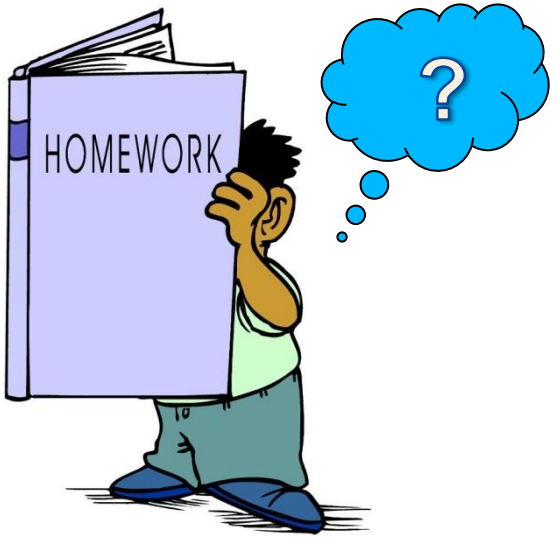
The survival probability



Exercise 2

Trapping

- Create a program which generates a 2 dimensional lattice of size 1000 x 1000. In this lattice place at random positions a number of trap molecules with concentration *c*. Place one particle at a random position on the lattice and let it perform a random walk as in the previous exercises. In this walk you will not place a time restriction, i.e. you will not declare a specific number of steps. The walk will stop when the particle falls on a trap. The time required for this is the trapping time. Perform 100000 runs, save the trapping times and make the distribution of these times.
- Run this program for $c = 10^{-2}$ and 10^{-3}. Put both distributions on the same graph. Describe your conclusions.



Exercise 2

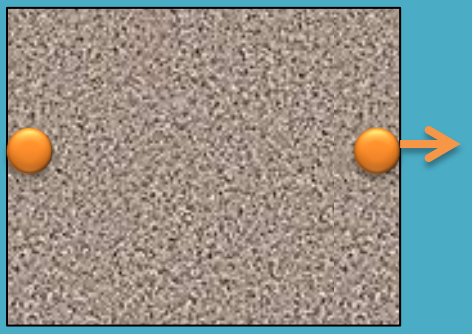
- **boundary conditions!!**
- *periodic boundaries* ⇒ *System* → ∞

Exercise 2

- **boundary conditions!!**
- *periodic boundaries* ⇒ *System* → ∞

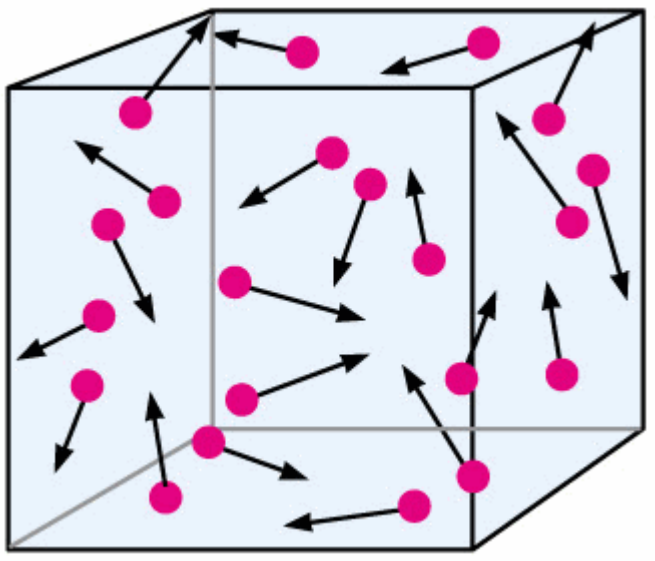
```
if (x==N)   then x = 0

if (y==N)   then y = 0
```

Wrapping the system



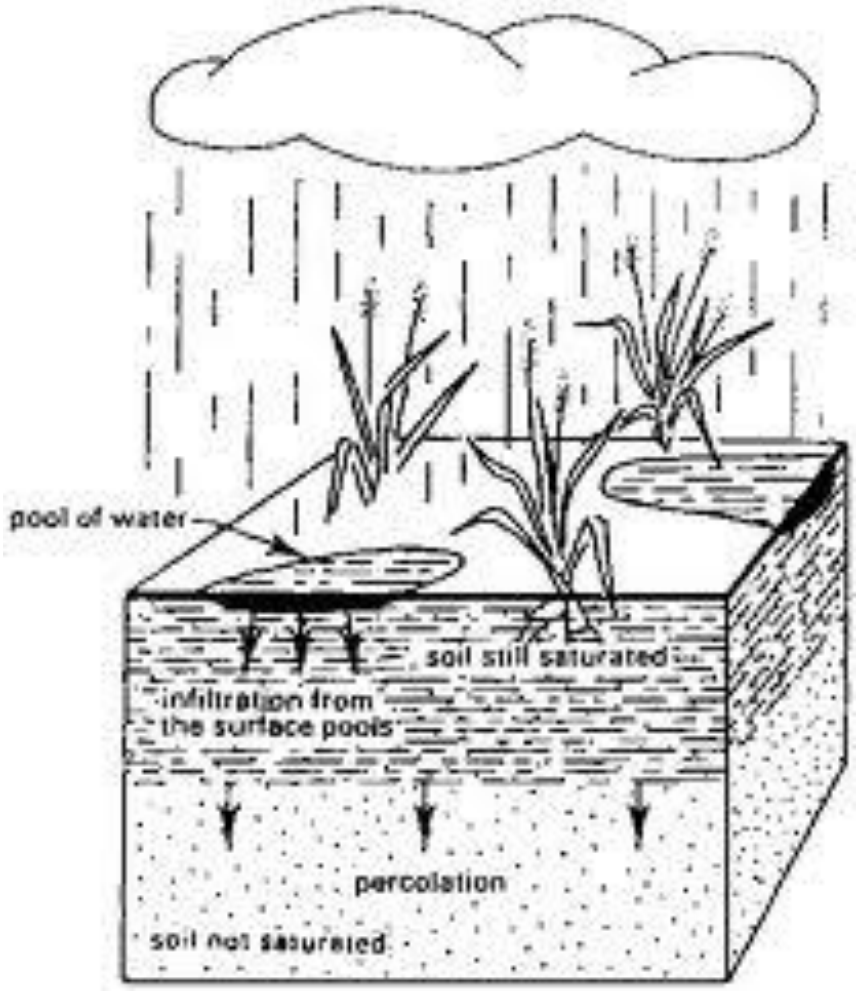
Exercise 2

- **boundary conditions!!**
  - *Finite System*



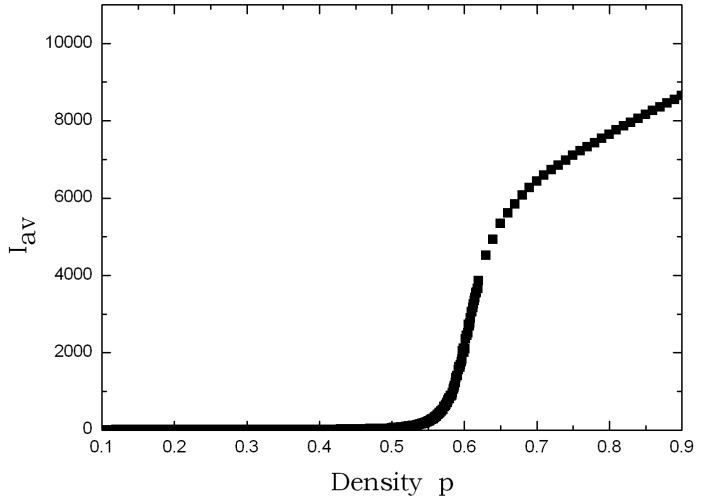
Let's take a break ..

Percolation in lattices



Percolation in lattices

- The Basic tool describing amorphous materials
- We can study geometrical phase transitions



Percolation in lattices

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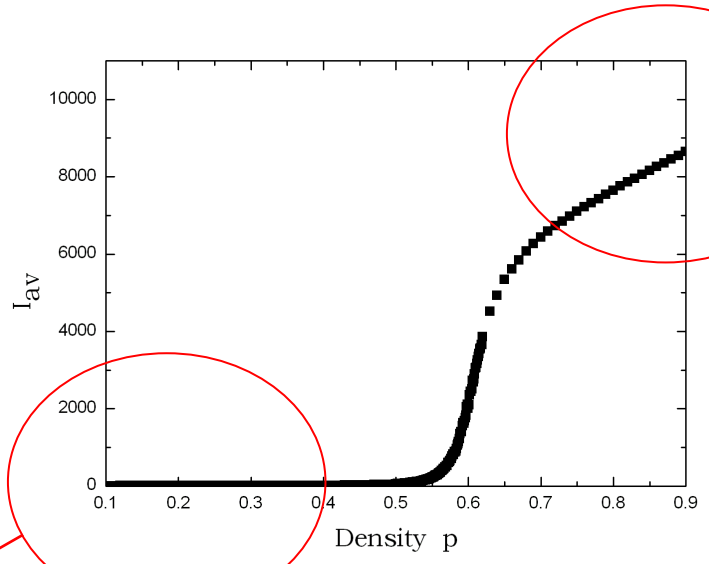
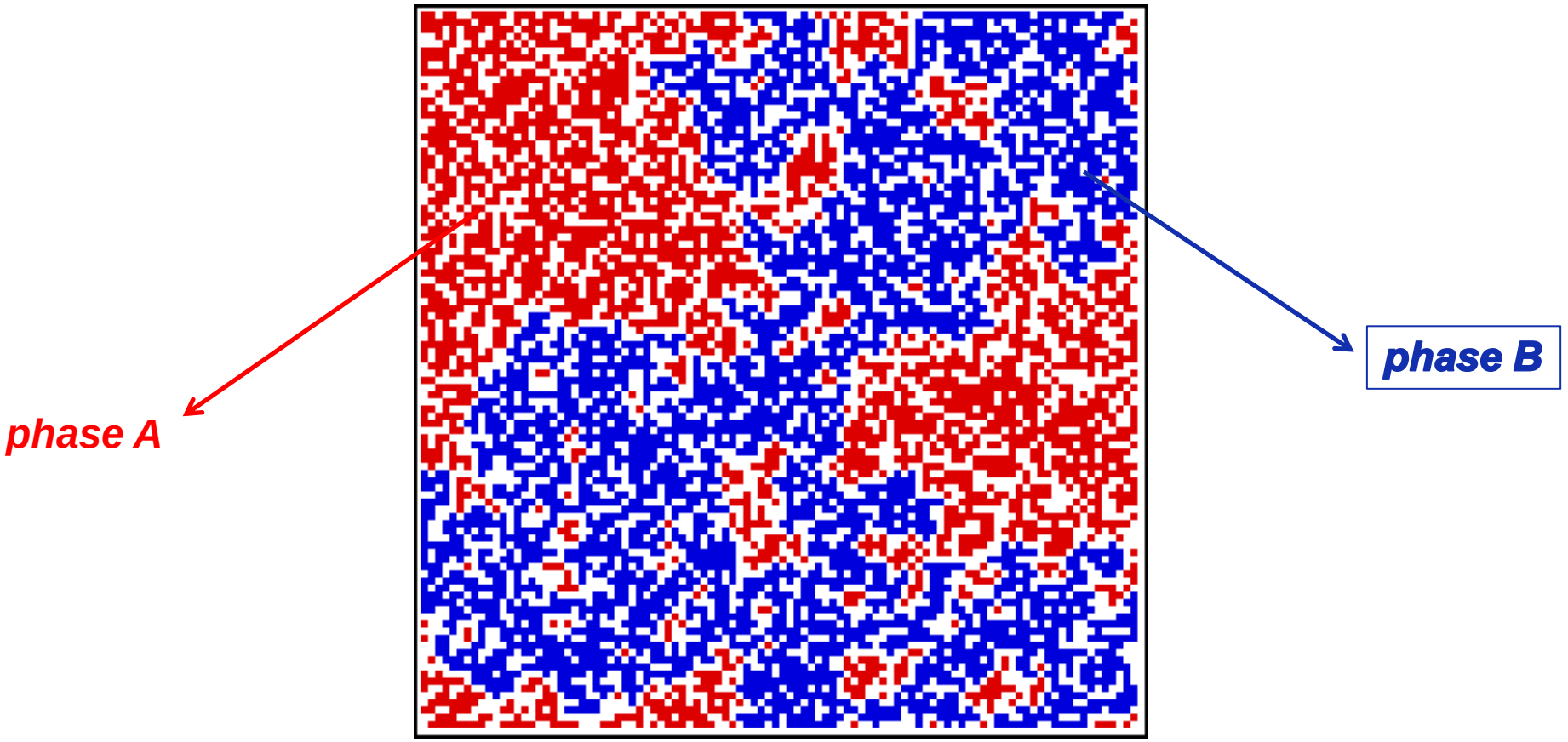


phase B

phase A

But what is a "phase transition" … ?

Percolation in lattices

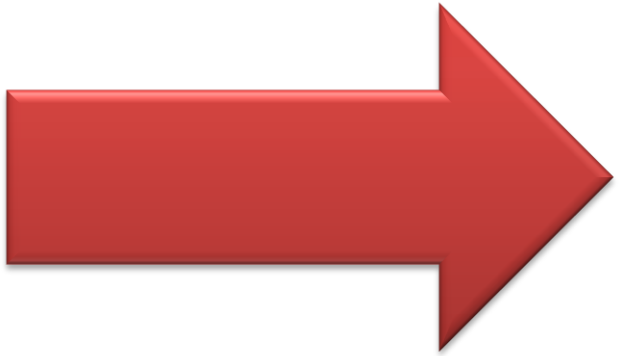


Percolation in lattices

Different types of percolation:

Lattices:

- Square
- Triangular
- Hexagonal
- etc..

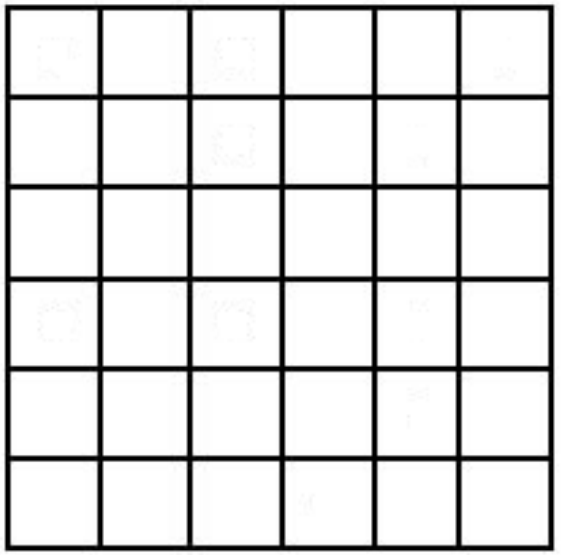


Types:

- Bond
- Site

Percolation

a brief description

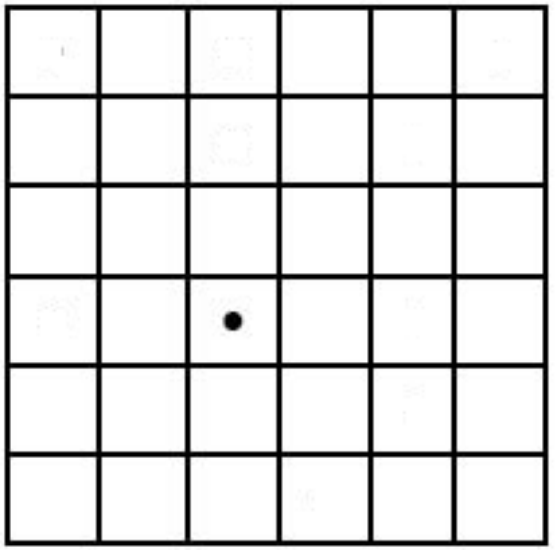


Percolation

a brief description

p = 1/36 = 2.7%

1-p = 35/36 = 97.3%



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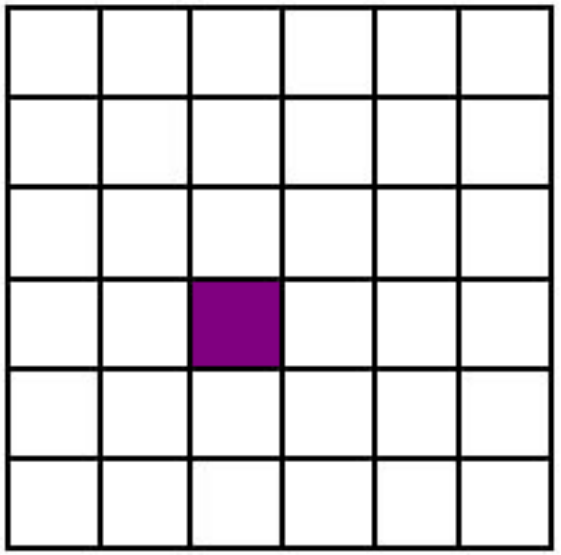
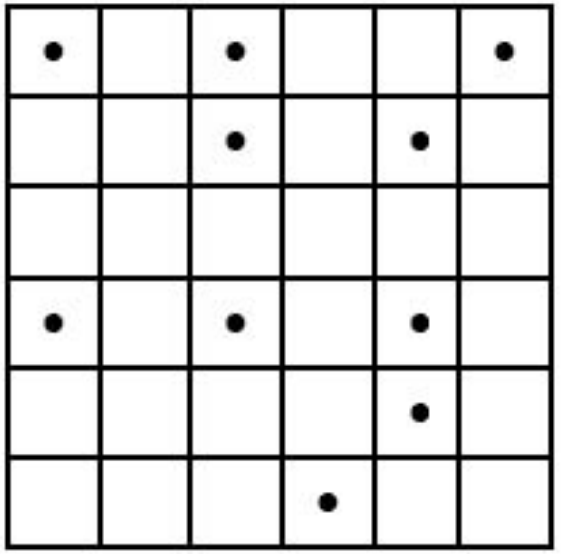


Percolation

a brief description

p = 10/36 = 27.7%

1-p = 26/36 = 72.3%



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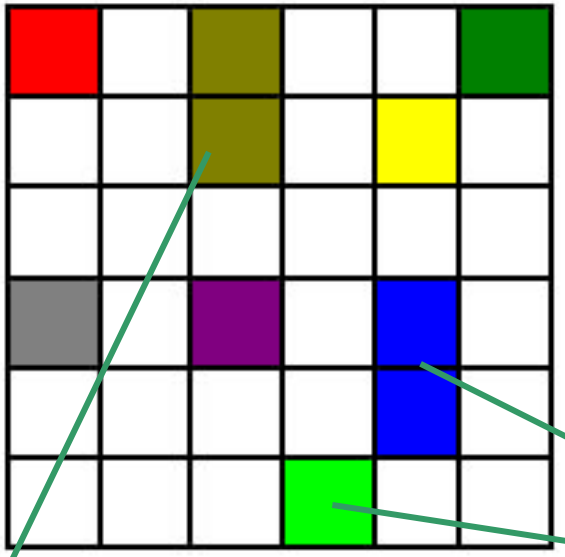


When two sites are connected to each other, they merge a “cluster”.

square lattice : We can say that two sites are connecting only to the four basic directions.

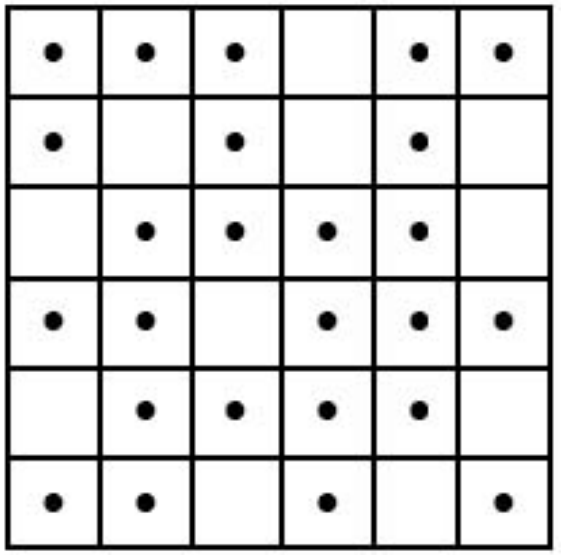
(right-left-up-down)

Percolation

a brief description

p = 25/36 = 69.4%

1-p = 11/36 = 30.6%



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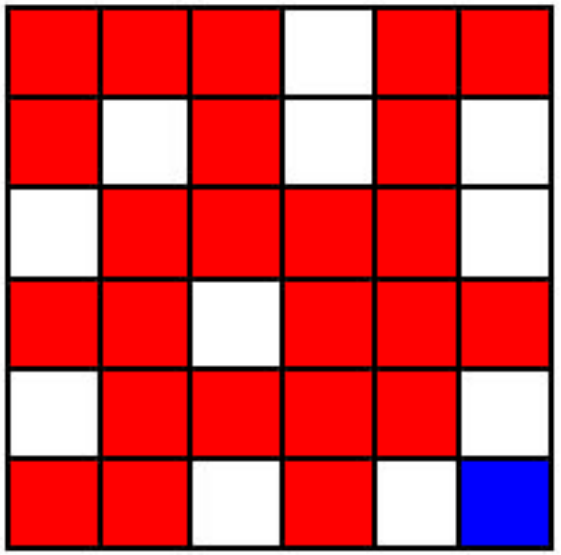
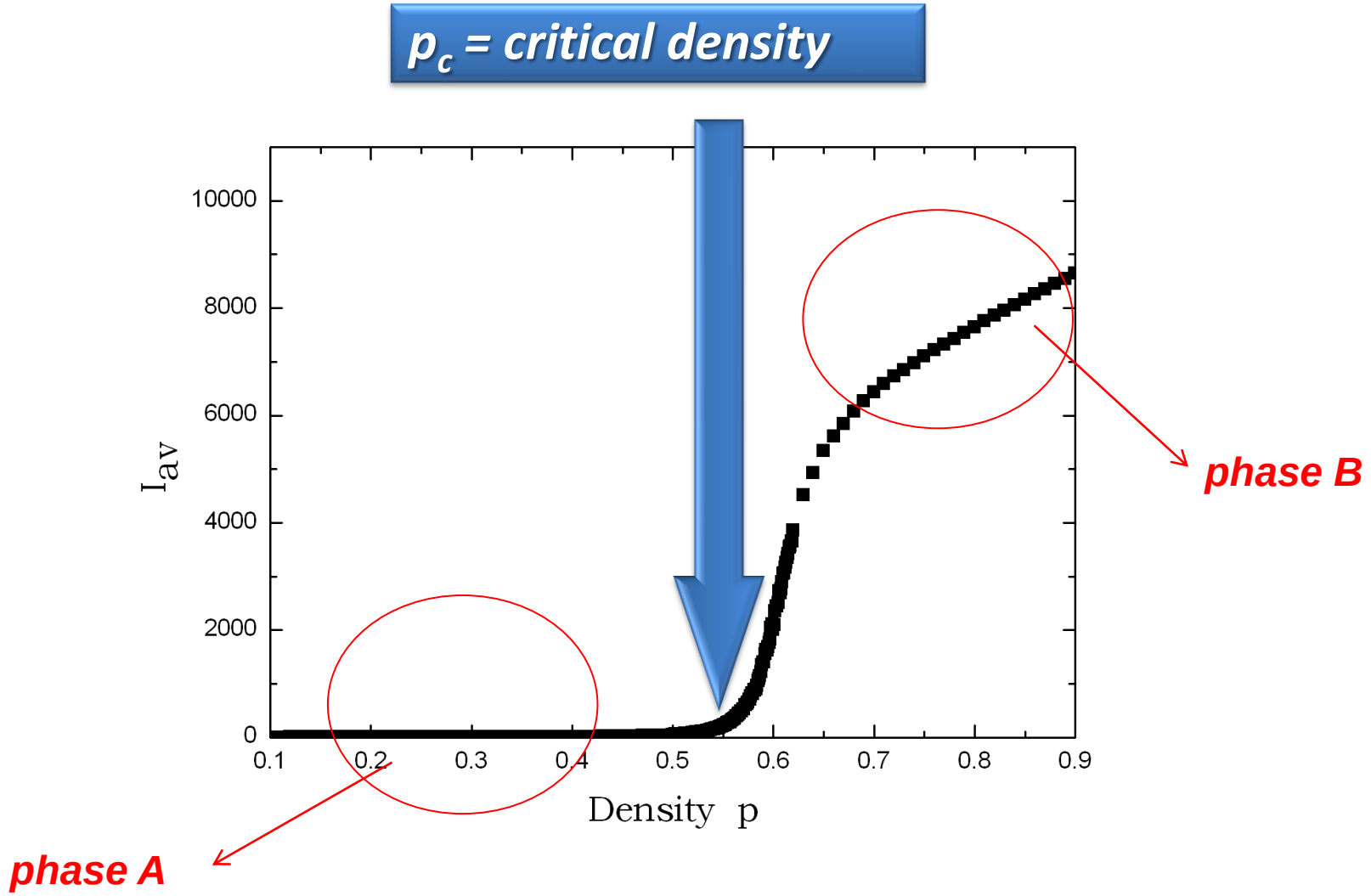


Spanning Cluster

When one cluster is spanning the system from the one end to the other.

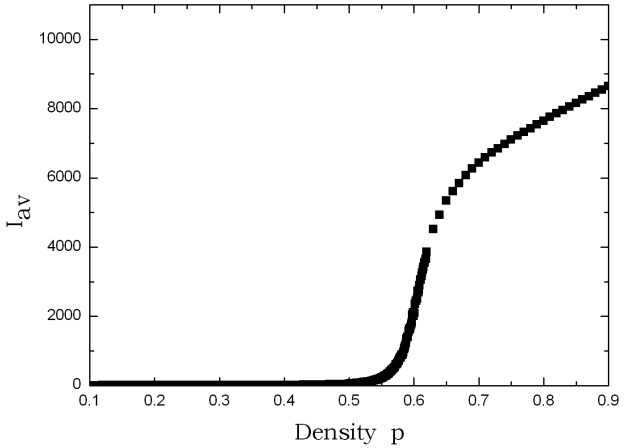
Percolation

a brief description



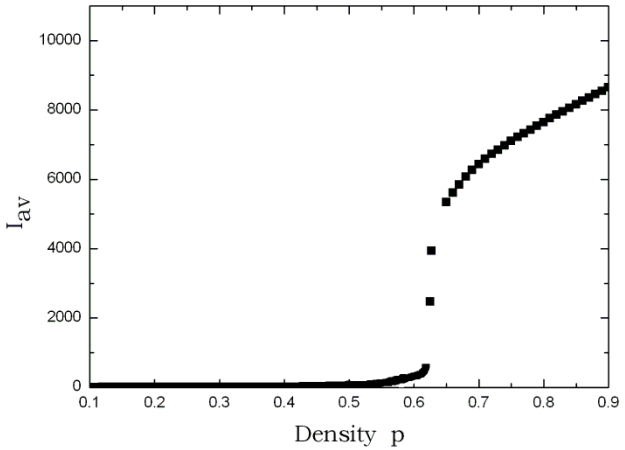
Percolation

a brief description



continuous phase transition

p_c : critical density



discontinuous phase transition

(1st Order)

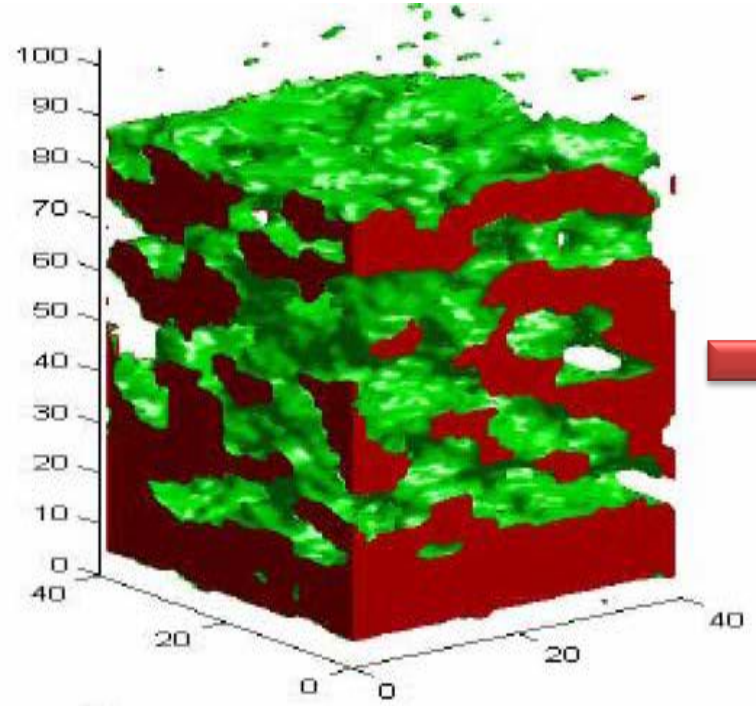
Percolation

a brief description

Lattice	**p_c (site percolation)**	**p_c (bond percolation)**
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**

Percolation

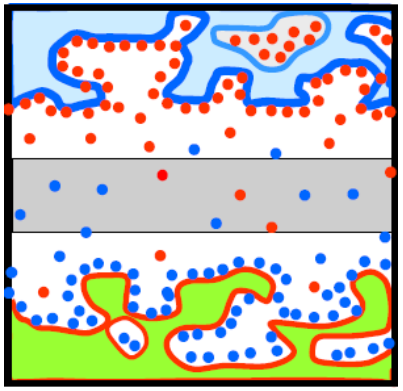
in materials

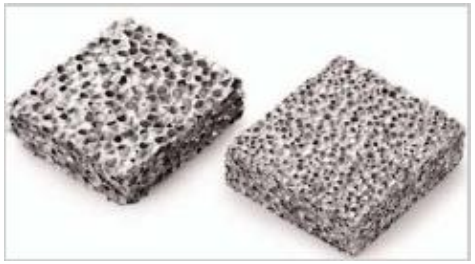


Organic Photovoltaic

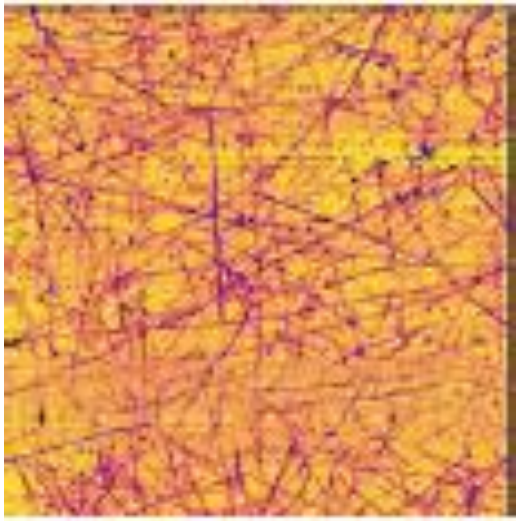
Percolation

in materials





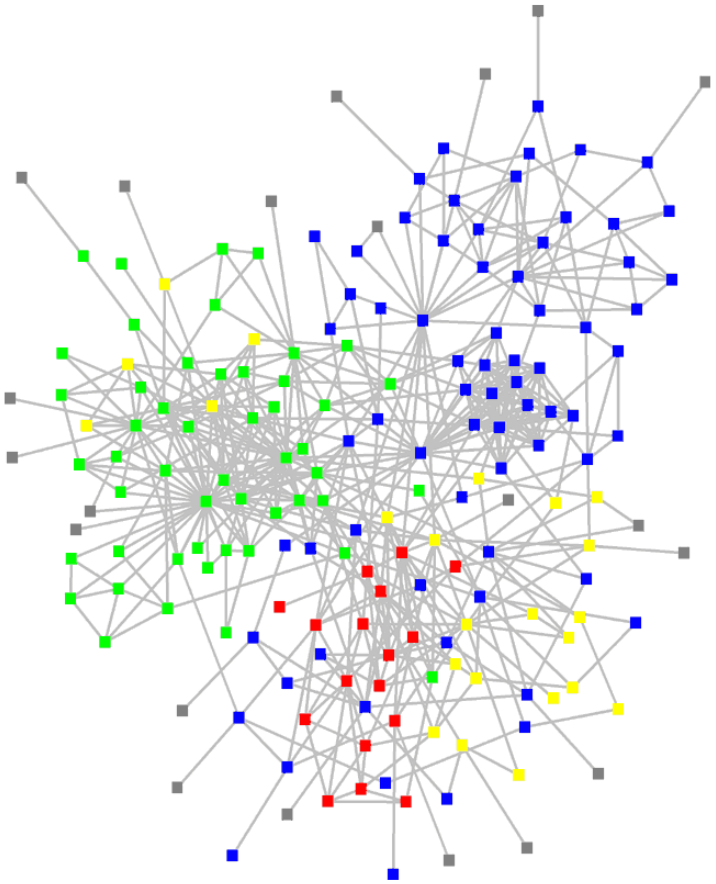
Super-Capacitors



Bio-Sensors

Percolation

in real life



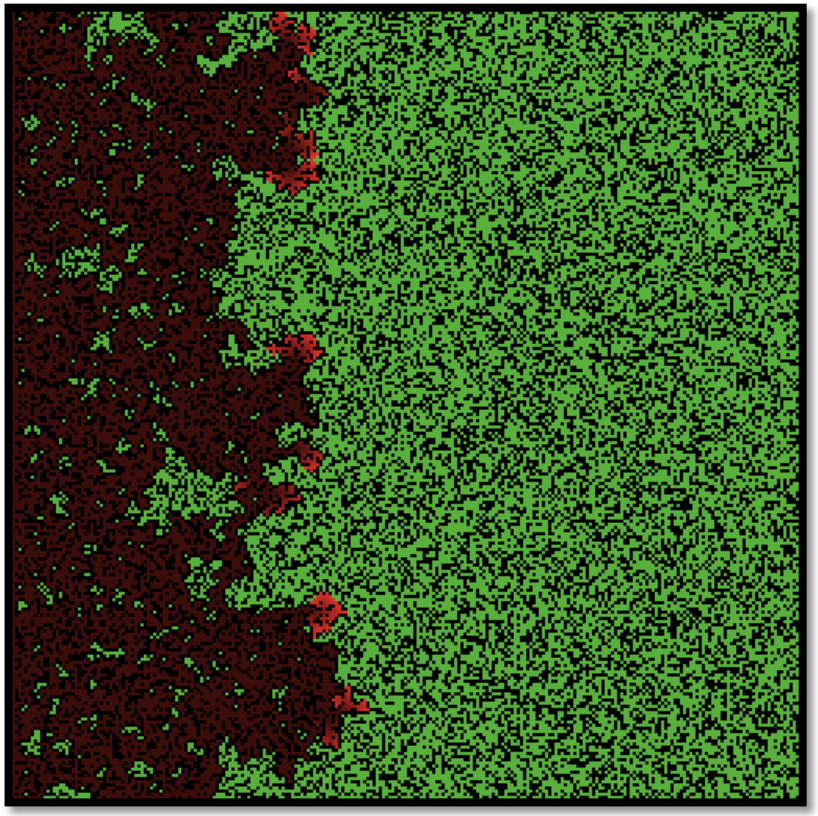
Spread of a disease

or

information

Percolation

in real life



Forest fire

Oil in a porous material

Percolation

in the computer!

The Hoshen-Kopelman Labeling Algorithm

- Developed in 1976 by Hoshen and Kopelman

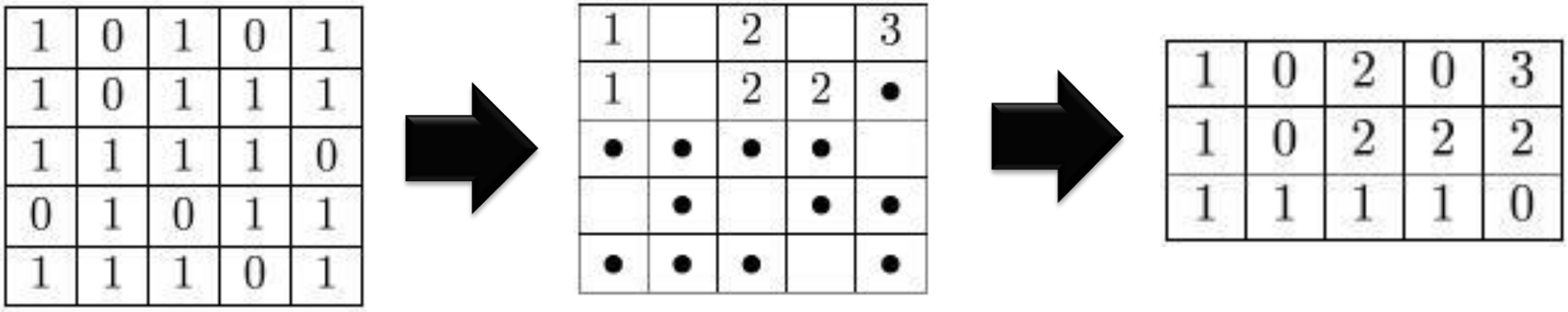
- Advantages
  - simple
  - fast
  - no need of huge data files (the lattice is created on the fly)
  - uses less memory than other algorithms

Percolation

in the computer!

The Hoshen-Kopelman Labeling Algorithm

Each site has a label



We give to each site the label of the cluster that belongs

Percolation

in the computer!

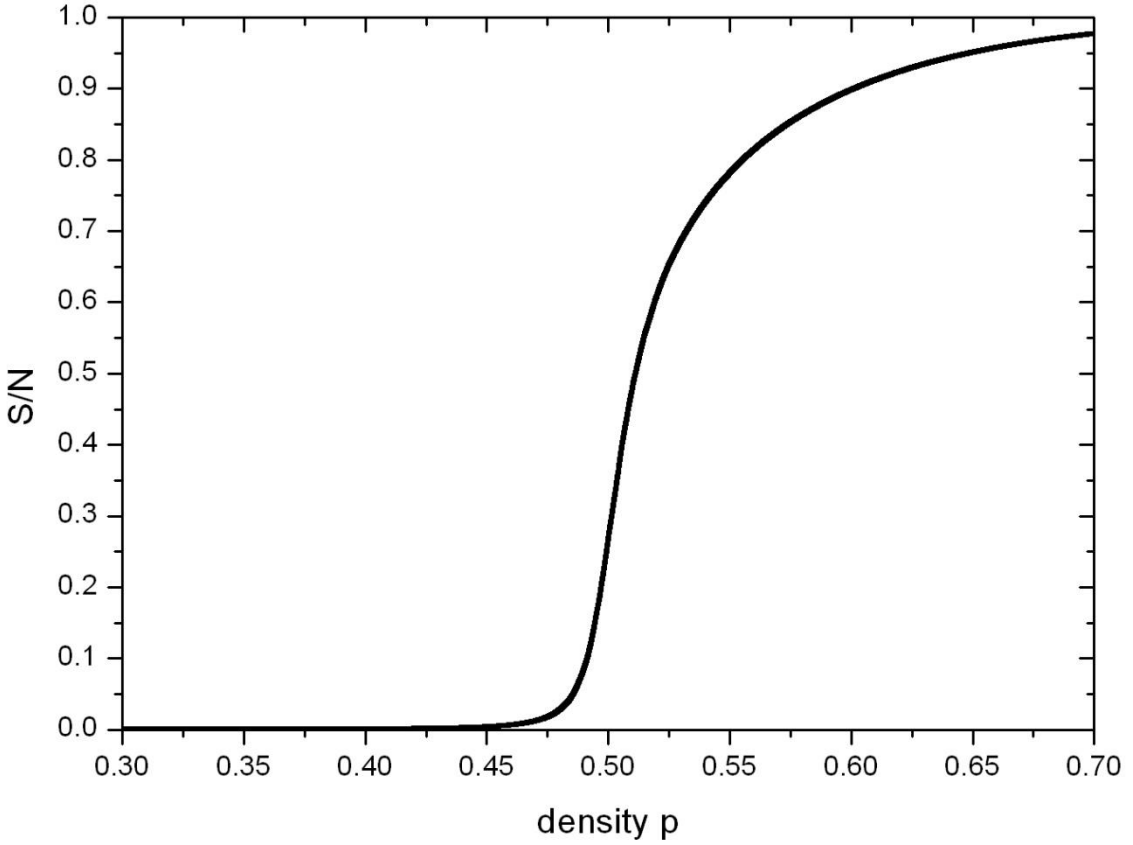
Calculating the mean cluster size *S*

$$S = \sum_{s=1}^{\infty} s\omega_s = \sum_{s=1}^{\infty} \frac{s^2 n_s}{\sum_{s=1}^{\infty} s n_s} = \frac{\sum_{s=1}^{\infty} s^2 n_s}{\sum_{s=1}^{\infty} s n_s}$$

Percolation

in the computer!

Plot of the mean cluster size ***S/N***



Percolation

in the computer!

Calculating the reduced mean cluster size S

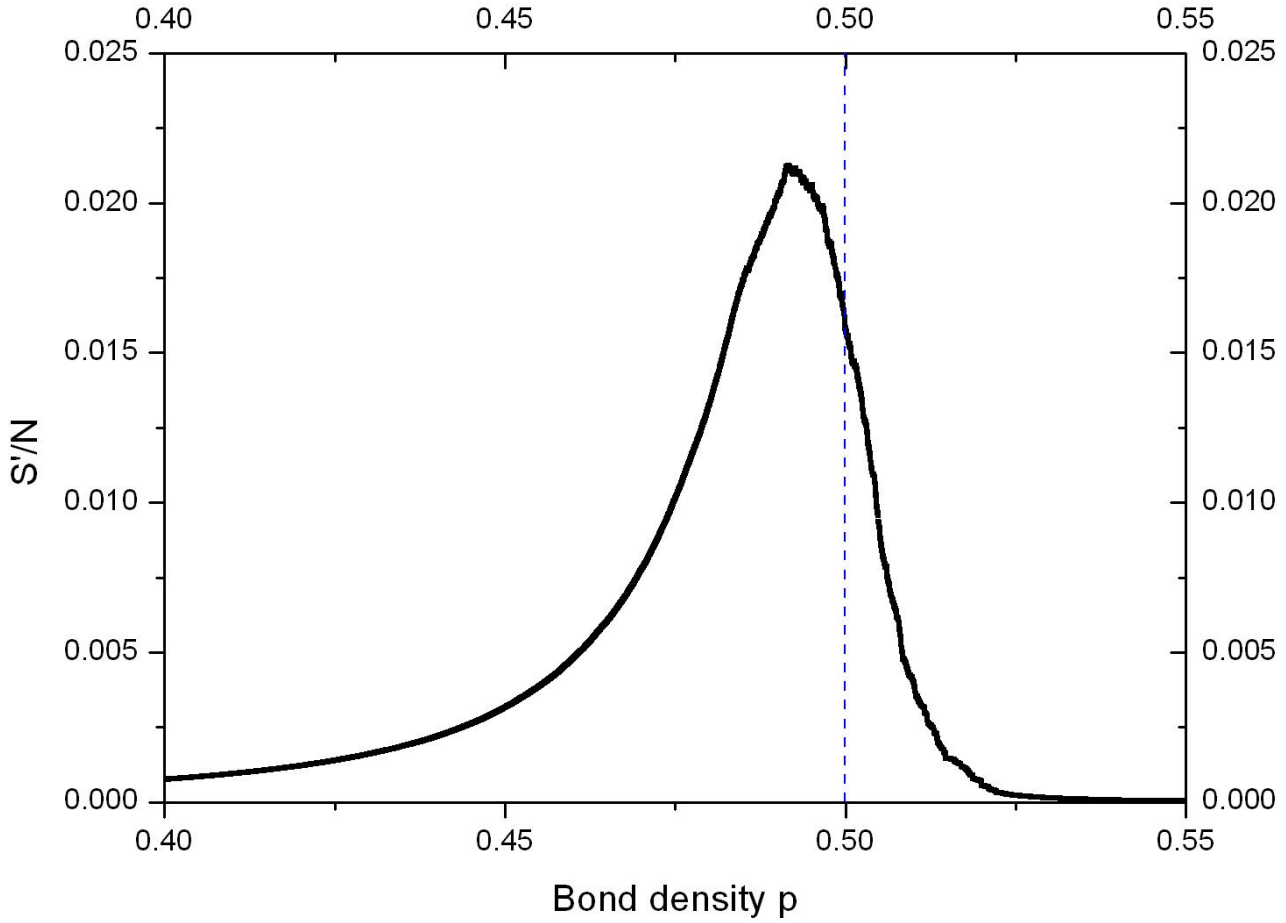
$$S = \sum_{s=1}^{\infty} s\omega_s = \sum_{s=1}^{\infty} \frac{s^2 n_s}{\sum_{s=1}^{\infty} s n_s} = \frac{\sum_{s=1}^{\infty} s^2 n_s}{\sum_{s=1}^{\infty} s n_s}$$

…without the maximum cluster

Percolation

in the computer!

Plot of the reduced mean cluster size S^{-1}/N



Percolation

in the computer!

Calculating the probability of one site to belong to the spanning cluster

$$P_{\max} = \frac{m_{\max}}{pN^2}$$

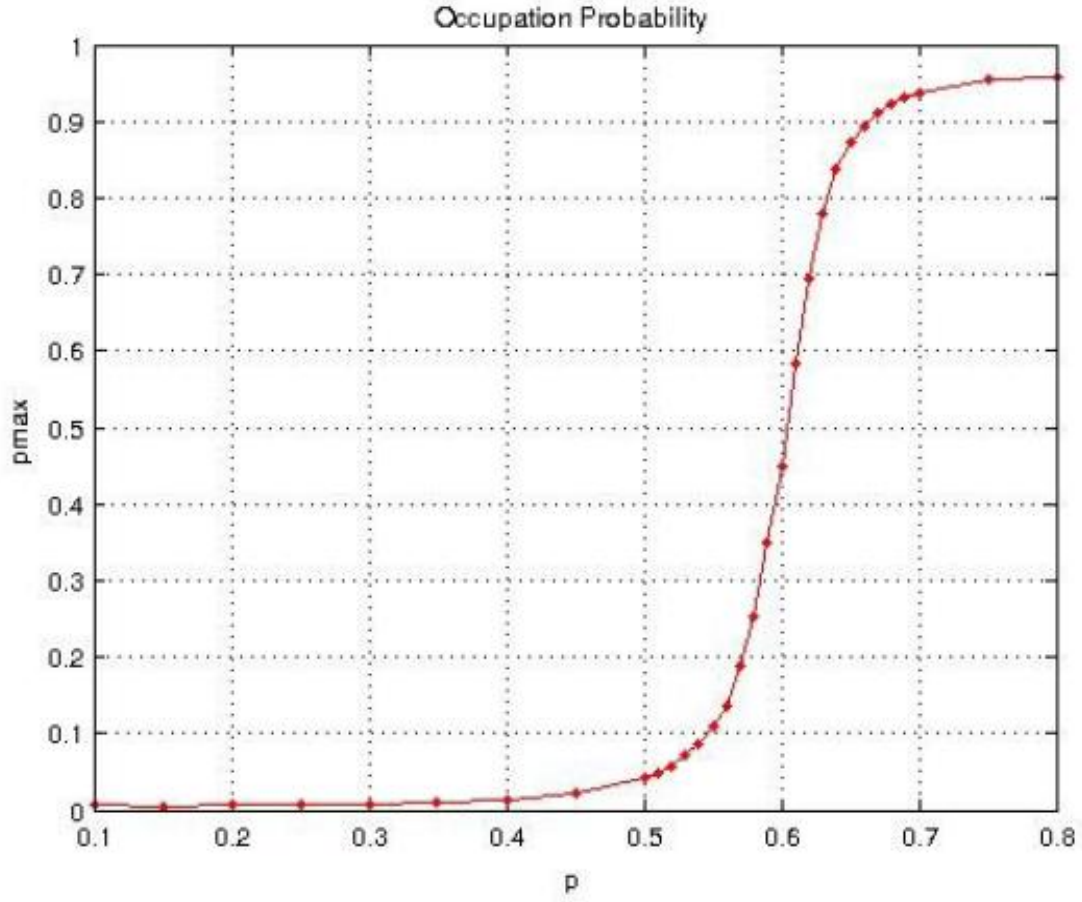
The size of the maximum cluster (in sites)

The total number of the sites that belong to a cluster.

Percolation

in the computer!

Plot of the probability of one site to belong to the spanning cluster



Percolation

in the computer!

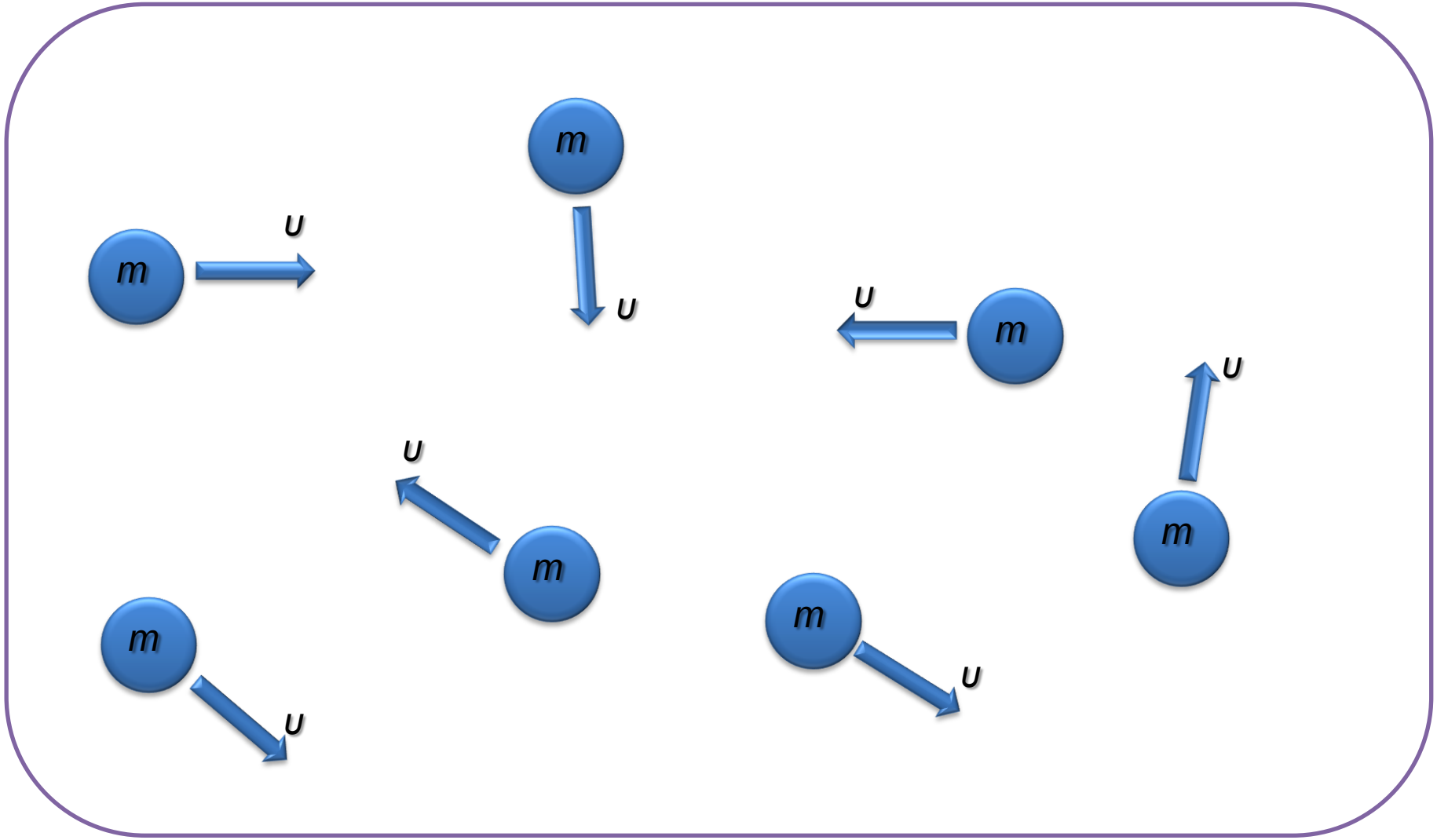
the critical exponents

$$I_{\alpha\nu}(p) = k\left|p - p_c\right|^{-\gamma}, p < p_c$$

$$I'_{\alpha\nu}(p) = k'\left|p - p_c\right|^{-\gamma'}, p > p_c$$

$$P_{\infty}(p) = k^{n}\left|p - p_c\right|^{-\beta}$$

molecular dynamics



molecular dynamics

- N-body problem
- interactions
- equations of motion
- dimensionless units
- We investigate:
  - velocities
  - energies
  - potentials
  - boundary conditions

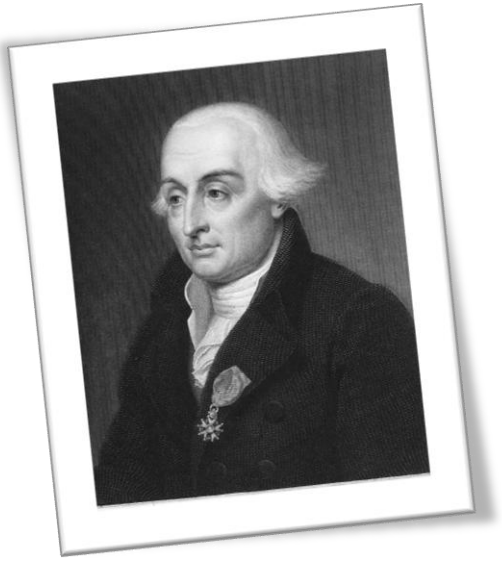
molecular dynamics

From

$$\vec{F} = \frac{d\vec{p}}{dt}$$

To

$$\frac{\partial L}{\partial q} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right) = 0$$



molecular dynamics

The Lennard-Jones potential

$$\phi(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} + \left(\frac{\sigma}{r}\right)^{6}\right]$$

which describes the interaction potential between two atoms A and B which are at distance r.

we assume units in which $\sigma = \varepsilon = 1$.

for more information...

- *visit:*

- http://icoscis.physics.auth.gr
- http://kelifos.physics.auth.gr/COURSES/courses.html

- *or e-mail:*

- **icoscis@physics.auth.gr**

for more information…

- *Or search for .. :*

1. D.P. Landau and K. Binder, “A Guide to Monte Carlo Simulations in Statistical Physics”, Cambridge University Press, 2000
2. Yaneer Bar-Yan, “Dynamics of complex systems”, Addison – Wesley, 1997
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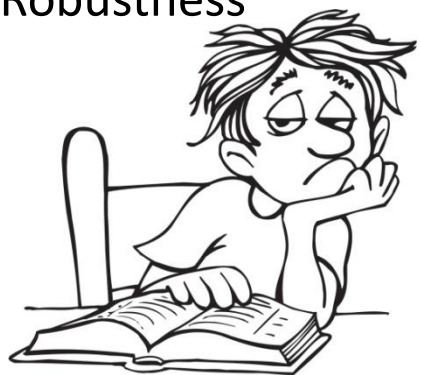

Find my presentation here:

http://db.tt/fyLDtDz5

Thank you for your attention!!