The Percolation problem: Solution with smart simulations

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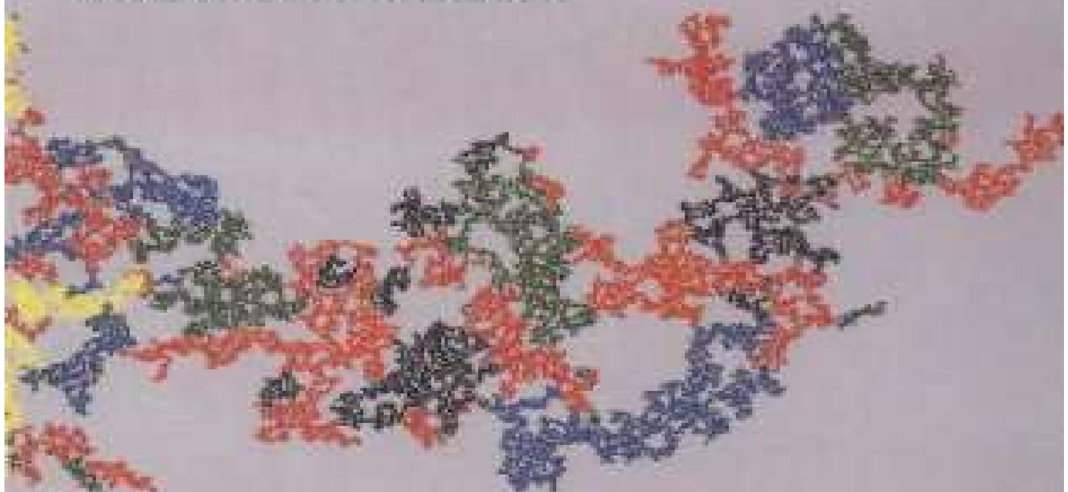
The percolation problem

Introduction to PERCOLATION THEORY

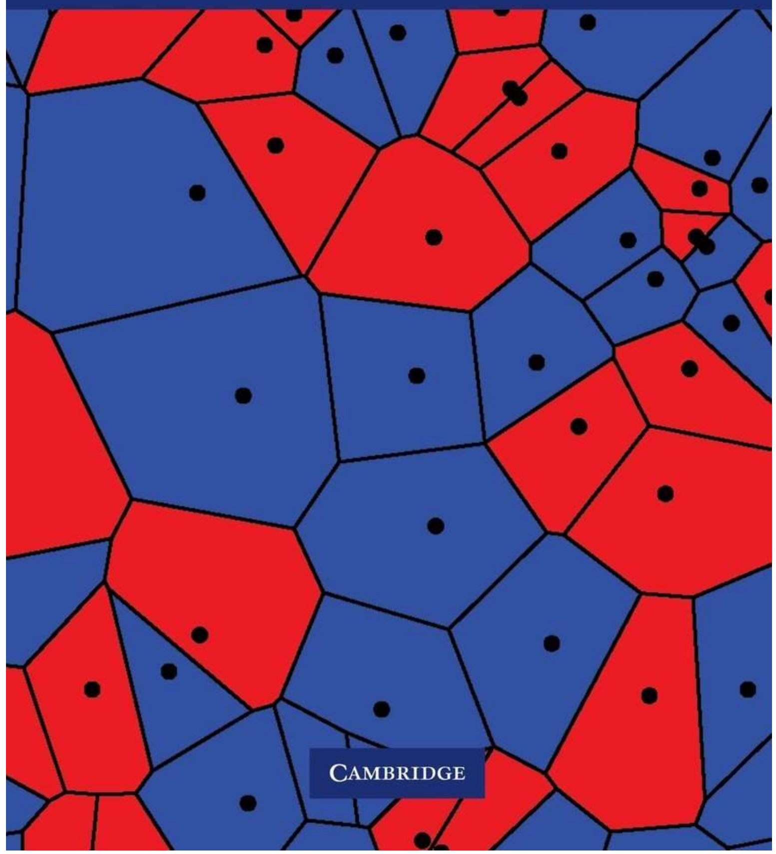
Revised Second Edition



DIETRICH STAUFFER AND
AMNON AHARONY

PERCOLATION

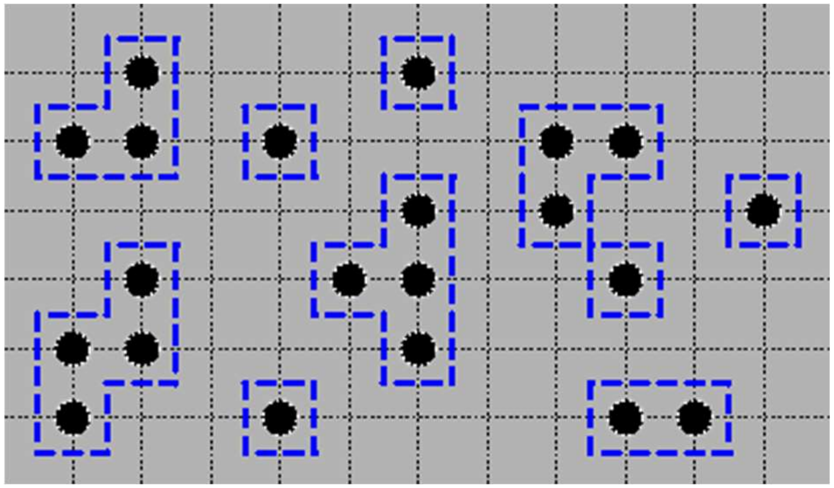
Béla Bollobás *and* Oliver Riordan

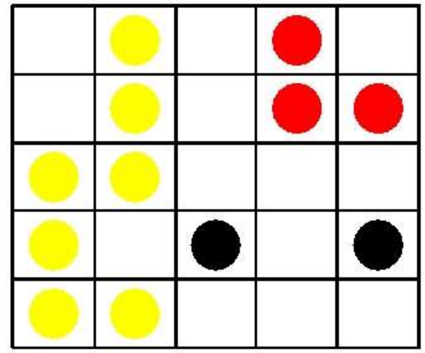


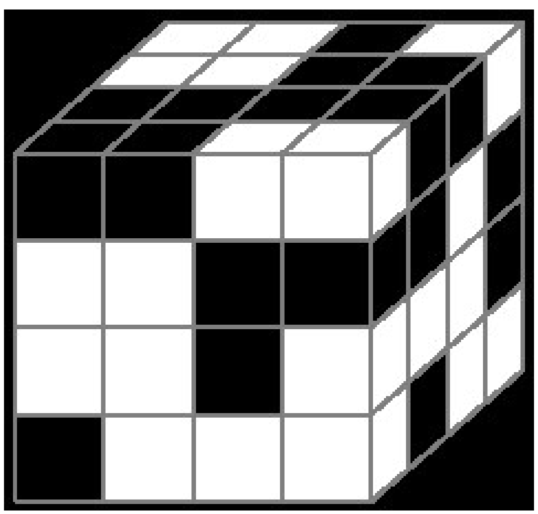
CAMBRIDGE

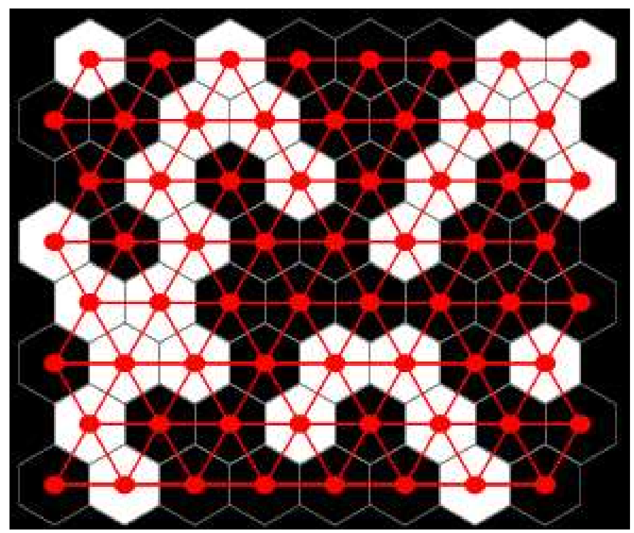
What is the problem?

- system made of 2 types of entities
- open/closed, true/false, conducting/insulating
- randomly mixed
- fixed ratio of open/closed, called “p”
- p in the range $0<p<1$
- adjacent entities of same type form clusters
- clusters depend on topology
- can be on lattice sites or on lattice bonds



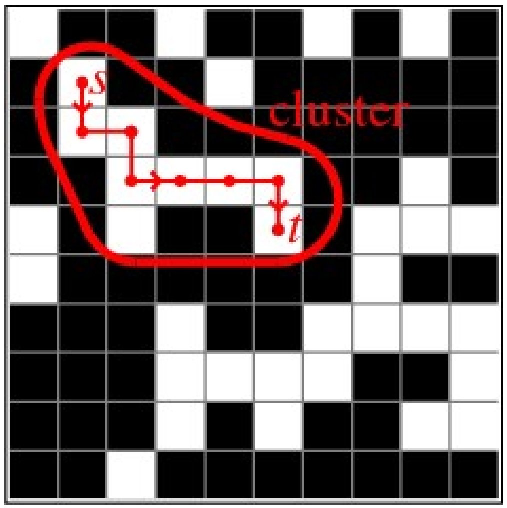




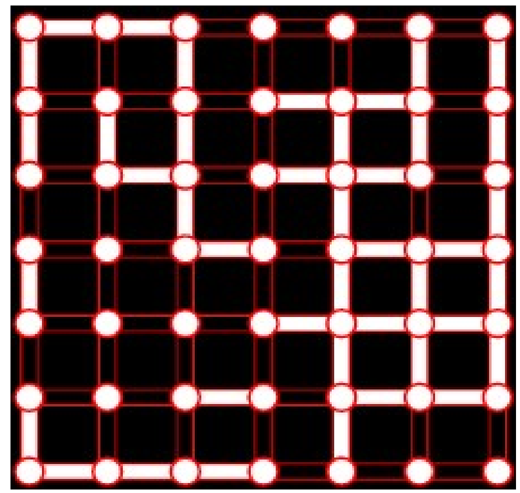


Site or bond percolation

site

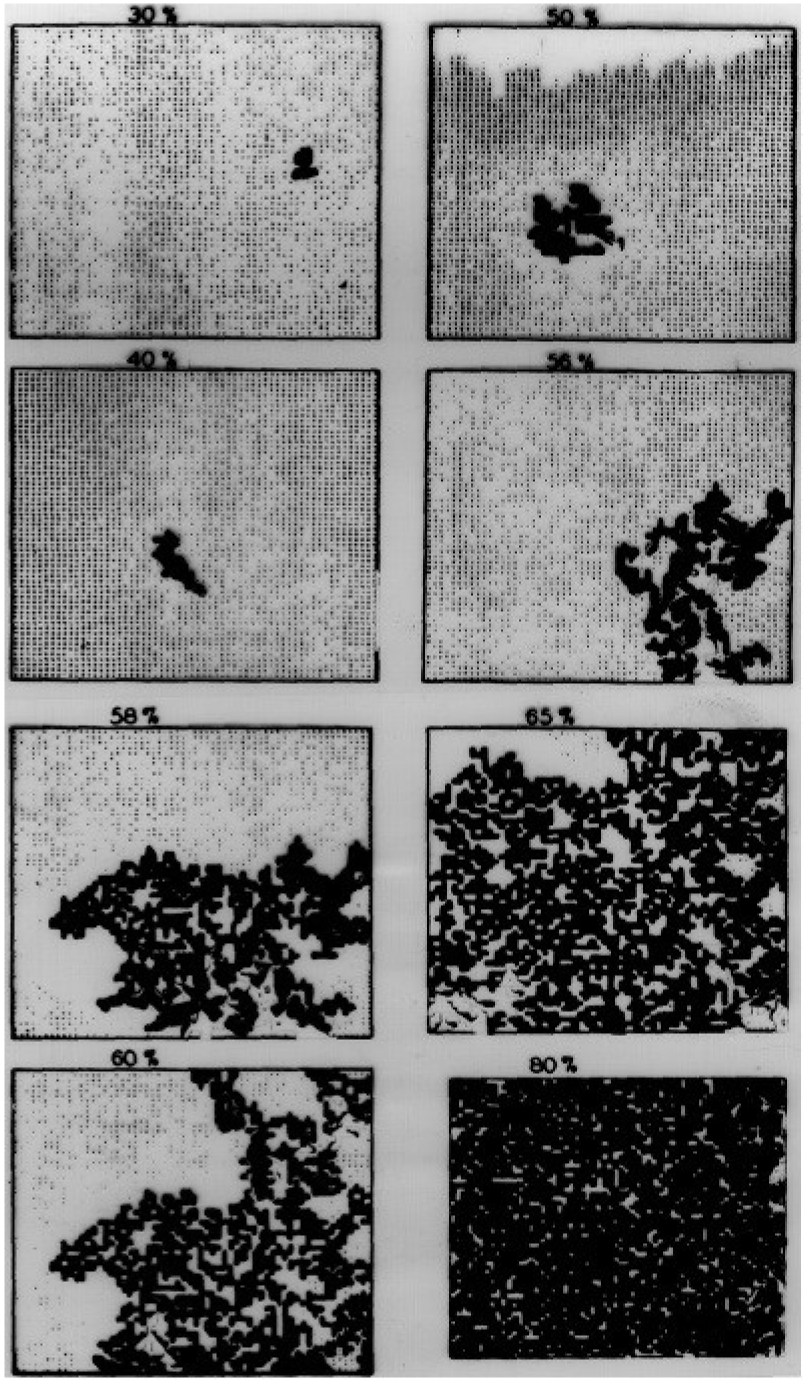


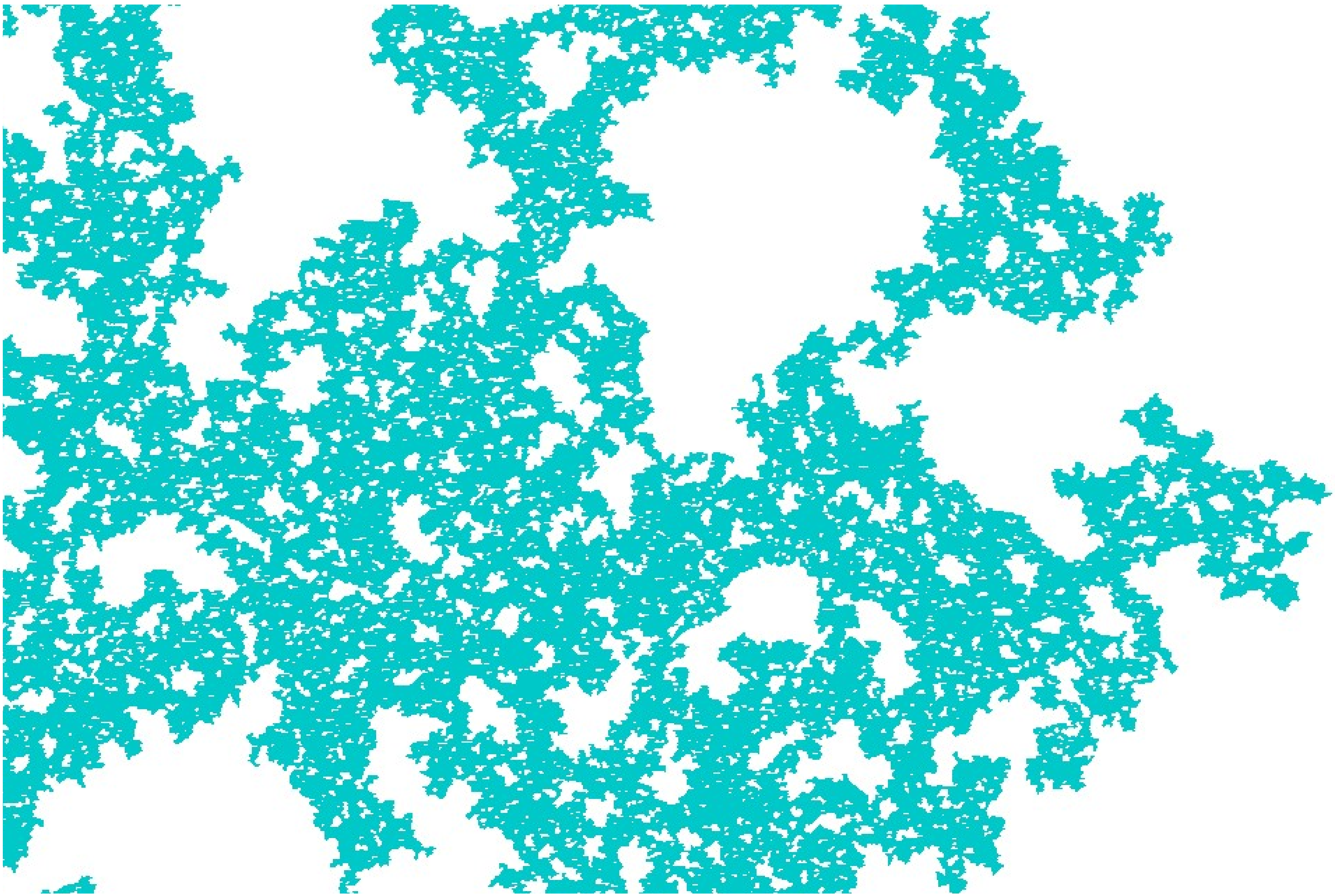
bond

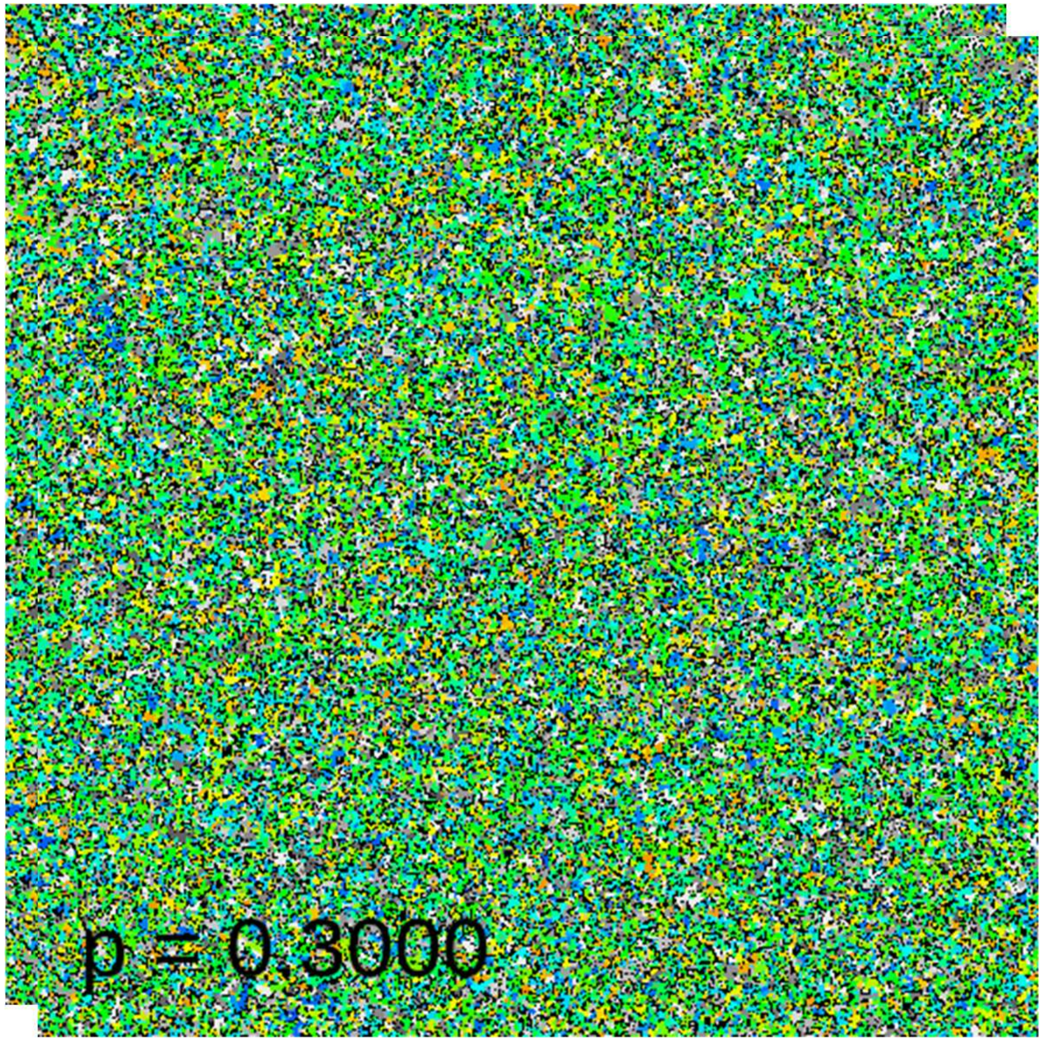


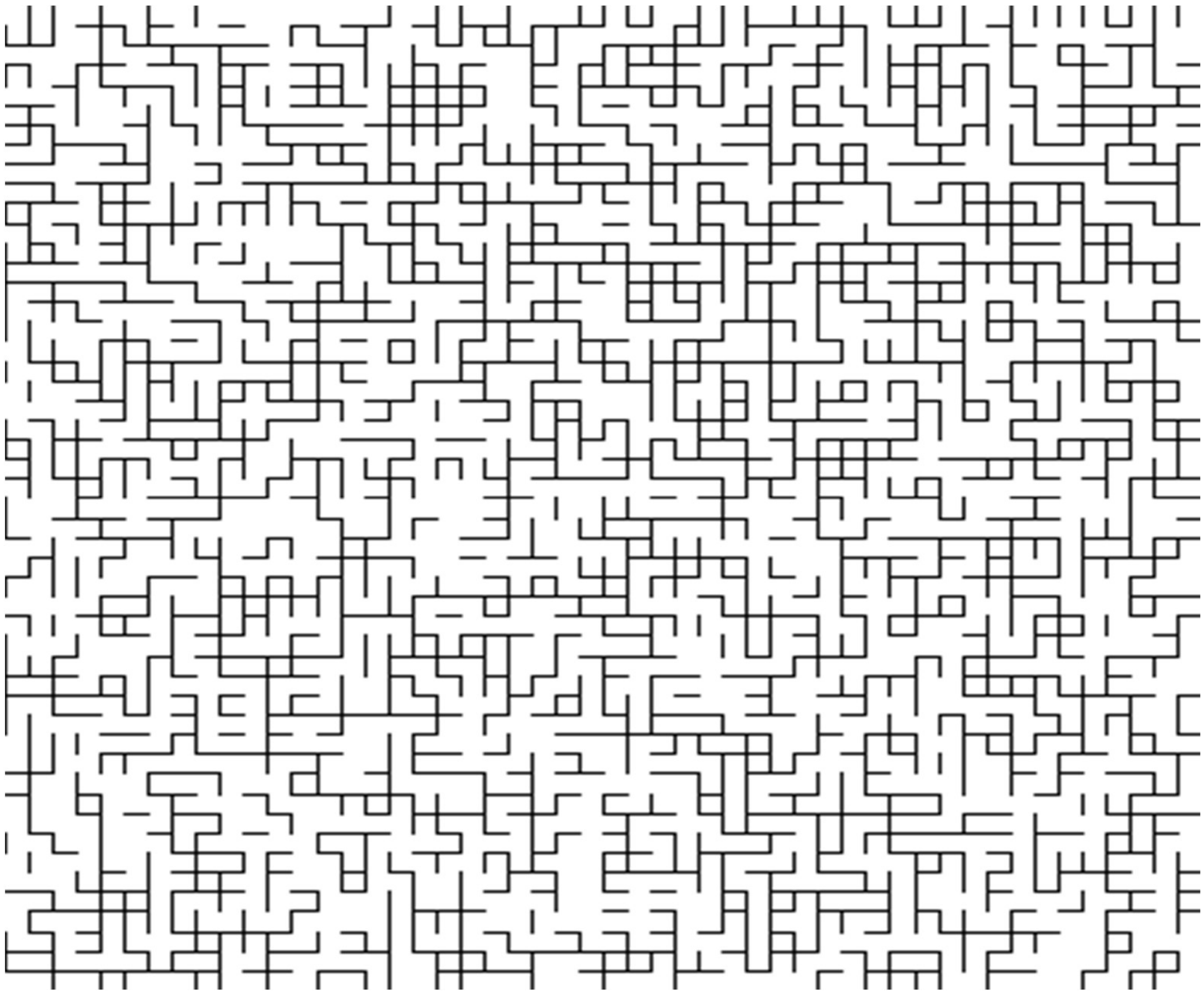
Percolation phase transition

- focus on largest cluster only
- size increases abruptly at the critical point
- system goes through a phase transition from "insulating" to "conducting"
- 2nd order phase transition, $\Delta H=0$

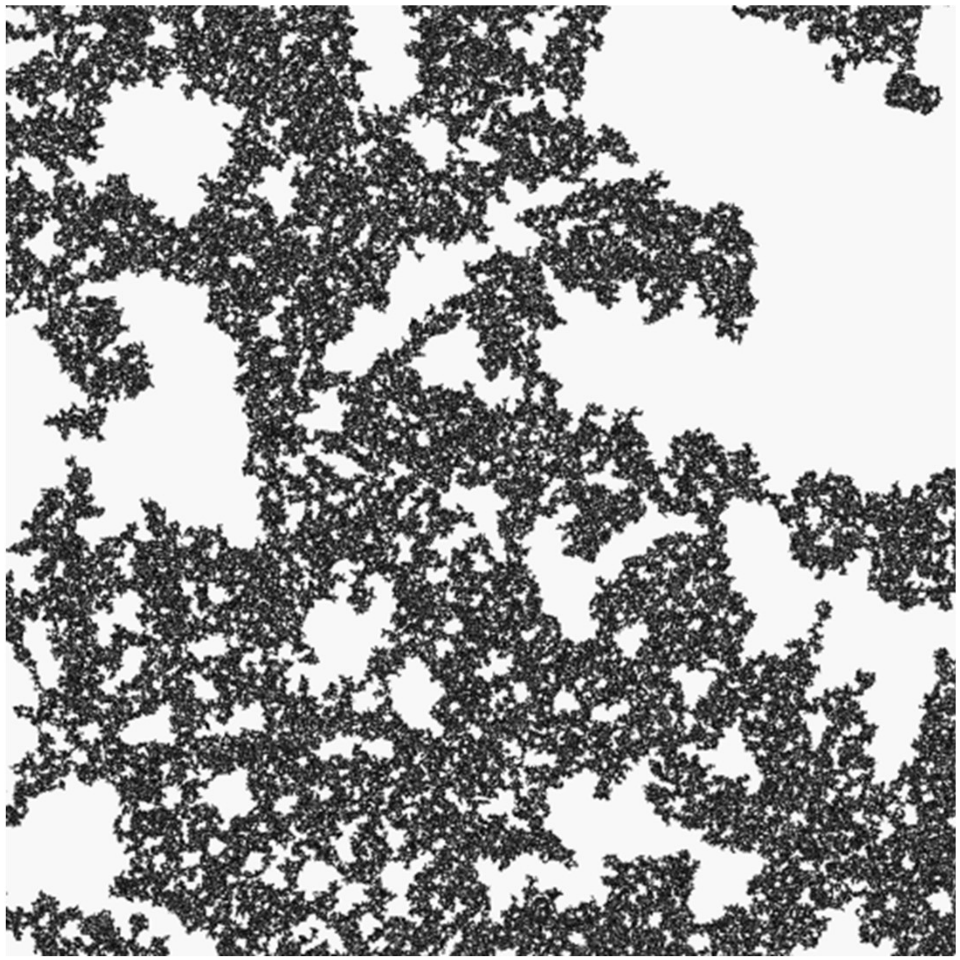

30 %
50 %
40 %
56 %
58 %
65 %
60 %
80 %




p = 0.3000

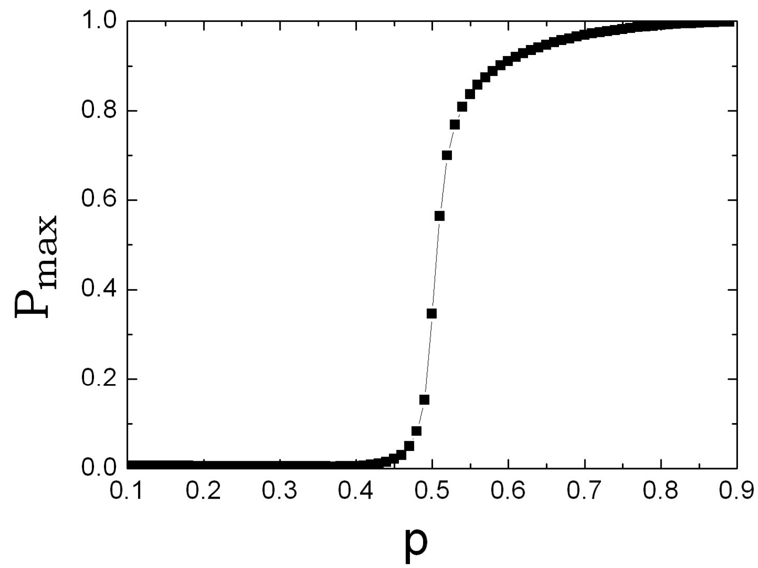


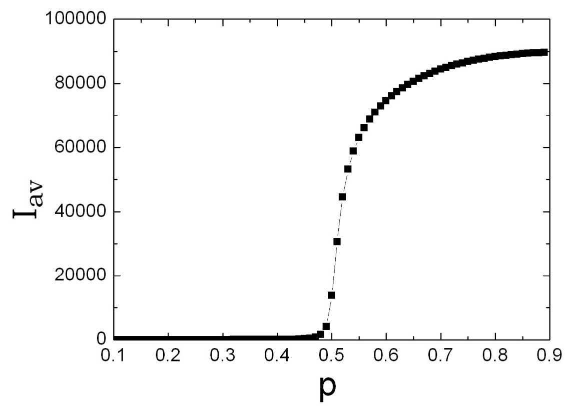
At criticality, p_c, the cluster ois a fractal

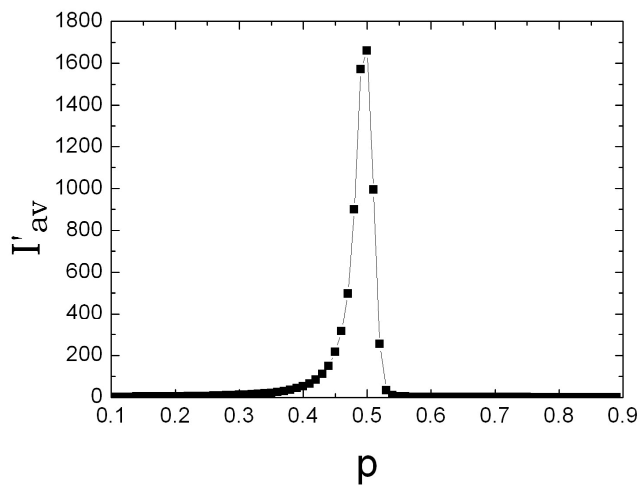


[Percolation simulation]

P(max)




100000
80000
60000
40000
20000
0
0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9
p
I_{av}


1800
1600
1400
1200
1000
800
600
400
200
0
0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9
p
I'_{av}

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

$$I_{\alpha v} = \sum_{m=1}^{m_{\max}} \frac{i_m m^2}{pN^2}$$

$$I_{av}^{'} = I_{av} - \frac{i_{\max} * m_{\max}^2}{p * N^2}$$

$$I'_{av} = \sum_{m=1}^{m-m_{max}} \left(\frac{i_{\mathrm{m}} \cdot m^2}{p \cdot N^2} \right)$$

How can we estimate p_c?

- several techniques have been developed
- square lattice (site percolation) p_c =0.5927……
- cannot be proven analytically
- square lattice (bond percolation) p_c =0.5000
- simple cubic(site) p_c =0.3116…
- simple cubic (bond) p_c =0.2488…
- p_c strongly depends on the lattice type
- the more nearest neighbors, the lower the p_c

Cluster Multiple Labeling Technique (CMLT)

- sweep the lattice from one end to the other
- for every cluster that appears give a different index number
- everytime 2 clusters join, they become one cluster
- "brute force" method: go back and merge the index numbers of the 2 clusters into 1 index number only. Need to sweep entire lattice
- CMLT method: need only a single sweep for the same job
- Invented by Hoshen (1976), called Hoshen-Kopelman algorithm

What happens when 2 clusters coalesce

- we need to add the 2 sizes into 1
- we change the label of the index, but NOT the index itself

Before the joining:

L(1)=1, L(2)=2, L(3)=3…..

After joining:

L(3)=2………

1	0	1	1	0	0	0	1	1	0	1	0	1	0	0	0	1	1	0	1
1	1	1	1	0	1	0	0	0	1	0	1	1	1	1	1	1	0	1	1
1	0	1	0	1	1	0	0	0	1	1	1	1	1	1	1	1	0	1	0
0	1	1	1	1	0	0	1	1	1	1	0	1	1	1	1	1	0	1	1
0	0	0	0	1	1	1	1	0	1	0	1	1	0	0	0	1	0	1	1
0	0	0	0	0	1	1	1	0	0	0	0	0	0	0	0	1	1	1	0
1	1	1	0	0	1	1	1	1	0	1	1	0	1	1	1	0	0	1	0
1	1	1	0	1	1	1	1	1	0	1	0	1	0	0	0	0	0	1	1
1	1	0	0	1	1	0	0	0	0	1	1	0	1	0	0	0	0	0	1
1	0	1	0	0	1	0	1	1	1	0	0	0	1	1	0	0	0	1	1
1	1	0	1	1	0	1	1	1	1	0	1	0	0	1	1	1	0	0	0
0	1	1	1	1	0	1	0	1	0	1	0	1	0	1	1	0	0	0	1
1	1	1	0	0	1	1	0	0	0	0	0	1	0	0	1	0	1	0	1
1	1	1	1	1	0	0	1	1	0	1	1	1	1	1	0	1	0	0	1
0	1	0	1	1	0	1	1	1	1	1	1	1	1	1	0	0	1	0	1
0	1	0	1	1	1	1	0	1	1	0	1	0	1	0	1	0	1	1	1
1	0	1	1	0	0	0	1	1	1	1	0	0	0	1	1	0	1	1	1
1	1	1	0	0	0	1	0	1	0	1	0	0	1	0	0	1	1	0	1
0	1	1	1	0	0	1	0	0	1	0	0	0	1	0	1	1	0	1	0
0	0	1	0	1	0	0	1	1	0	0	0	1	1	1	0	0	1	1	1

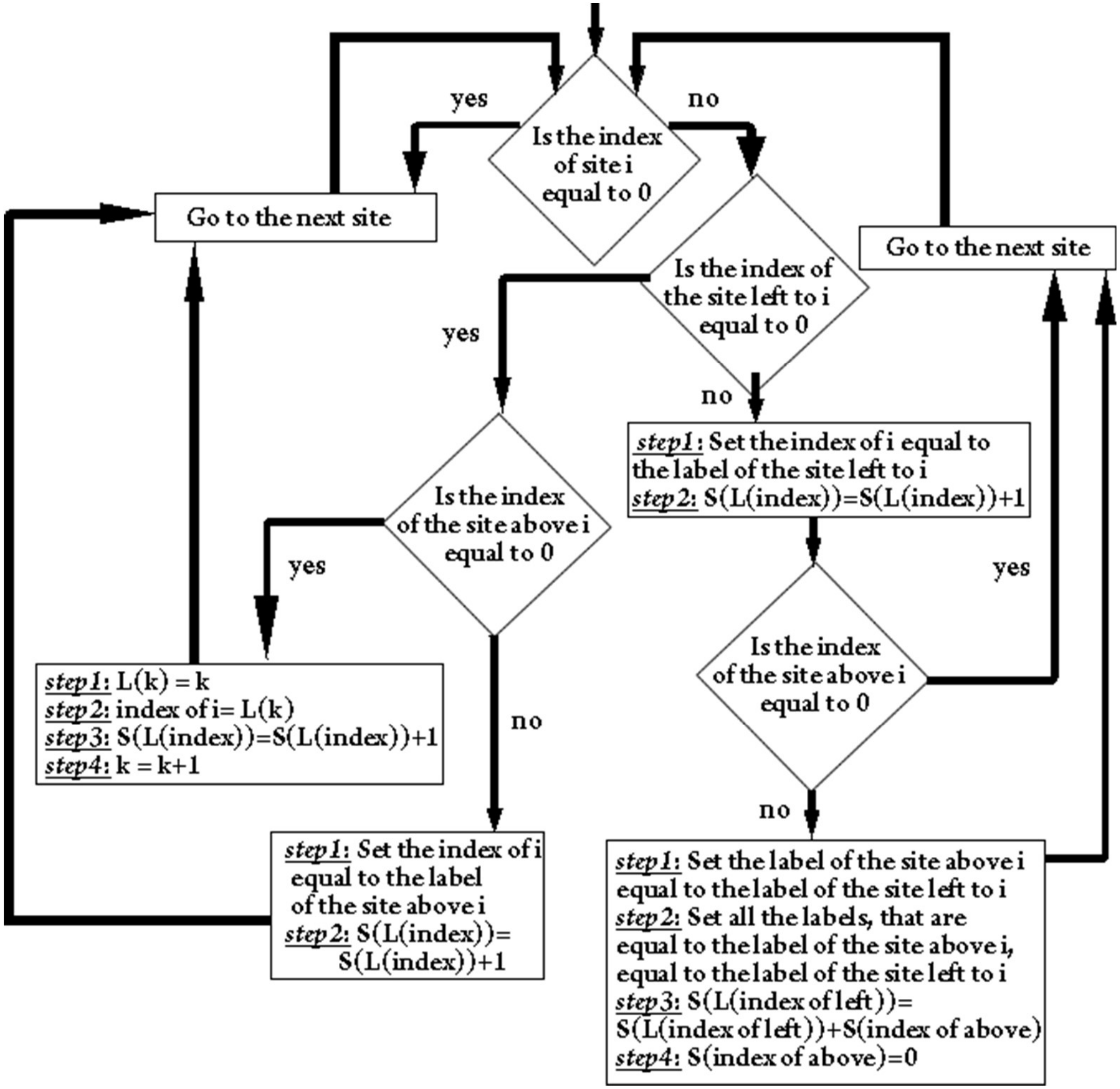
Part (a)

1	0	6	5	0	0	0	18	18	0	26	0	33	0	0	0	43	31	0	52
1	1	1	5	0	13	0	0	0	24	0	30	11	31	31	31	31	0	49	31
1	0	1	0	10	5	0	0	0	24	11	11	11	31	31	31	31	0	49	0
0	5	5	5	5	0	0	19	11	11	11	0	11	31	31	31	31	0	49	31
0	0	0	0	5	5	11	11	0	11	0	31	31	0	0	0	31	0	49	31
0	0	0	0	0	5	11	11	0	0	0	0	0	0	0	0	31	31	31	0
2	2	3	0	0	5	11	11	11	0	27	27	0	37	37	37	0	0	31	0
2	2	3	0	11	11	11	11	11	0	27	0	34	0	0	0	0	0	31	31
2	2	0	0	11	11	0	0	0	0	27	27	0	38	0	0	0	0	0	31
2	0	7	0	0	11	0	20	14	14	0	0	0	38	38	0	0	0	50	50
2	2	0	9	4	0	15	14	14	14	0	32	0	0	38	38	38	0	0	0
0	2	3	3	4	0	15	0	14	0	28	0	35	0	38	38	0	0	0	53
3	3	3	0	0	14	14	0	0	0	0	0	35	0	0	38	0	46	0	53
3	3	3	3	4	0	0	21	4	0	29	22	22	22	22	0	44	0	0	53
0	3	0	3	4	0	16	4	4	22	22	22	22	22	22	0	0	47	0	53
0	3	0	3	4	4	4	0	4	22	0	22	0	22	0	41	0	47	42	42
4	0	8	4	0	0	0	22	22	22	22	0	0	0	40	40	0	47	42	42
4	4	4	0	0	0	17	0	22	0	22	0	0	39	0	0	45	42	0	42
0	4	4	4	0	0	17	0	0	25	0	0	0	39	0	42	42	0	51	0
0	0	4	0	12	0	0	23	23	0	0	0	36	36	36	0	0	48	48	48

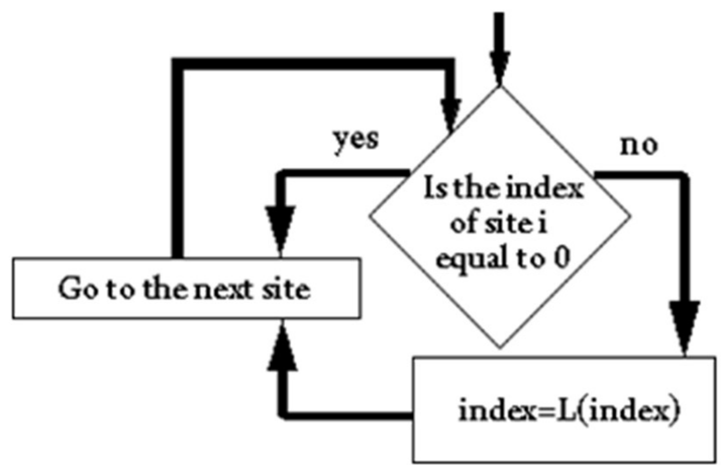
Part (b)

50	0	50	50	0	0	0	18	18	0	26	0	50	0	0	0	50	50	0	50
50	50	50	50	0	50	0	0	0	50	0	50	50	50	50	50	50	0	50	50
50	0	50	0	50	50	0	0	0	50	50	50	50	50	50	50	50	0	50	0
0	50	50	50	50	0	0	50	50	50	50	0	50	50	50	50	50	0	50	50
0	0	0	0	50	50	50	50	0	50	0	50	50	0	0	0	50	0	50	50
0	0	0	0	0	50	50	50	0	0	0	0	0	0	0	0	50	50	50	0
22	22	22	0	0	50	50	50	50	0	27	27	0	37	37	37	0	0	50	0
22	22	22	0	50	50	50	50	50	0	27	0	34	0	0	0	0	0	50	50
22	22	0	0	50	50	0	0	0	0	27	27	0	38	0	0	0	0	0	50
22	0	7	0	0	50	0	14	14	14	0	0	0	38	38	0	0	0	50	50
22	22	0	22	22	0	14	14	14	14	0	32	0	0	38	38	38	0	0	0
0	22	22	22	22	0	14	0	14	0	28	0	22	0	38	38	0	0	0	42
22	22	22	0	0	14	14	0	0	0	0	0	22	0	0	38	0	46	0	42
22	22	22	22	22	0	0	22	22	0	22	22	22	22	22	0	44	0	0	42
0	22	0	22	22	0	22	22	22	22	22	22	22	22	22	0	0	42	0	42
0	22	0	22	22	22	22	0	22	22	0	22	0	22	0	40	0	42	42	42
22	0	22	22	0	0	0	22	22	22	22	0	0	0	40	40	0	42	42	42
22	22	22	0	0	0	17	0	22	0	22	0	0	36	0	0	42	42	0	42
0	22	22	22	0	0	17	0	0	25	0	0	0	36	0	42	42	0	48	0
0	0	22	0	12	0	0	23	23	0	0	0	36	36	36	0	0	48	48	48

Part (c)

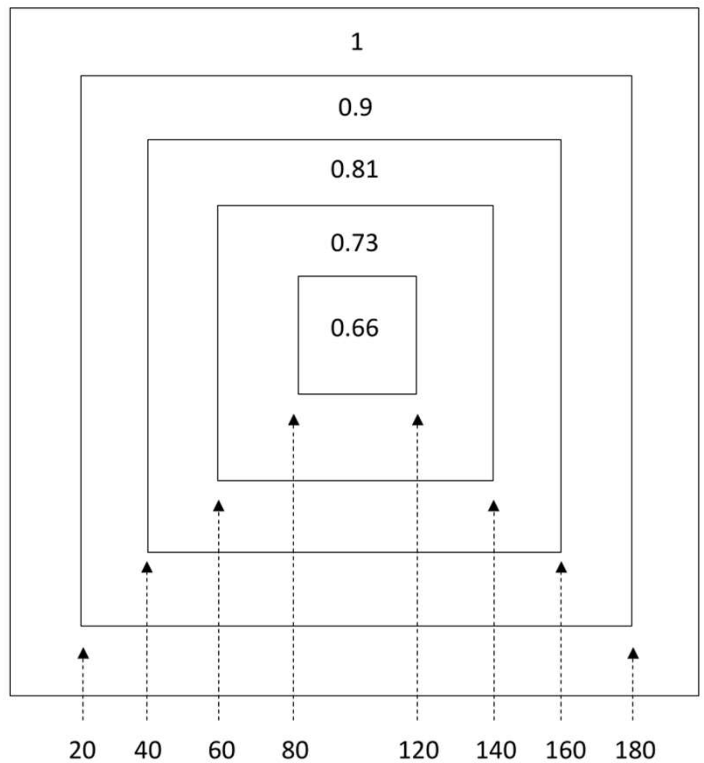


Is the index of site i equal to 0
yes
no
Go to the next site
Is the index of the site left to i equal to 0
Go to the next site
yes
no
step1: Set the index of i equal to the label of the site left to i
step2: S(L(index))=S(L(index))+1
Is the index of the site above i equal to 0
yes
no
yes
step1: L(k) = k
step2: index of i= L(k)
step3: S(L(index))=S(L(index))+1
step4: k = k+1
Is the index of the site above i equal to 0
no
no
step1: Set the index of i equal to the label of the site above i
step2: S(L(index))= S(L(index))+1
step1: Set the label of the site above i equal to the label of the site left to i
step2: Set all the labels, that are equal to the label of the site above i, equal to the label of the site left to i
step3: S(L(index of left))= S(L(index of left))+S(index of above)
step4: S(index of above)=0


yes
no
Is the index
of site i
equal to 0
Go to the next site
index=L(index)

http://kelifos.physics.auth.gr

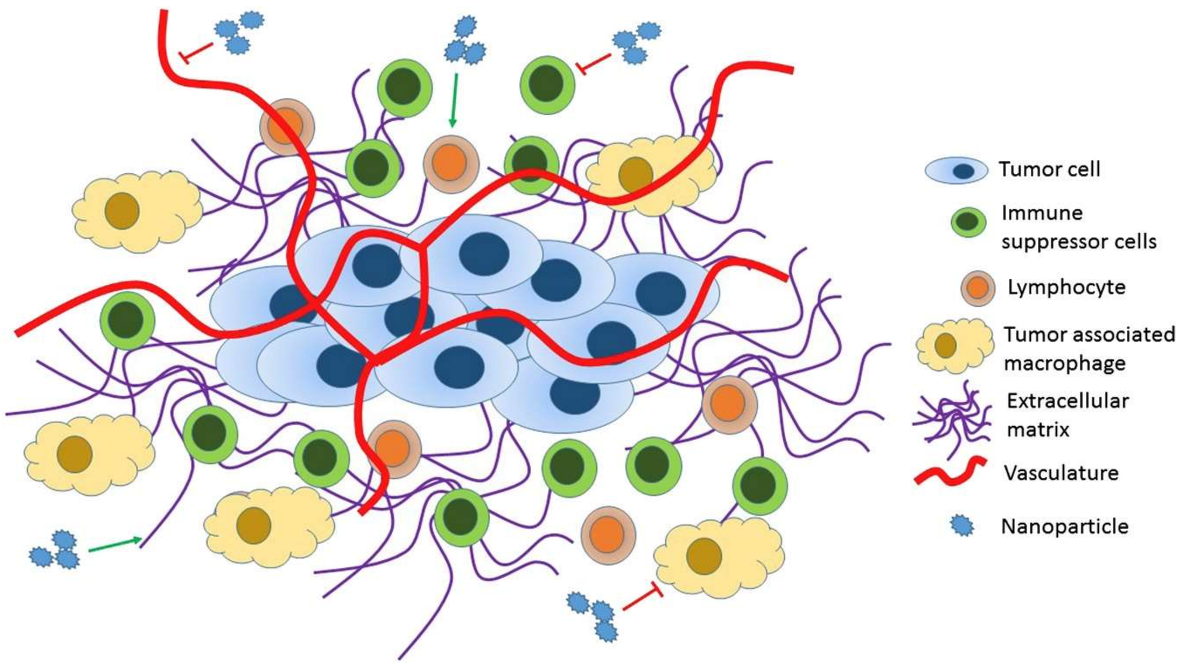
--->courses --->percolation


1
0.9
0.81
0.73
0.66
20
40
60
80
120
140
160
180

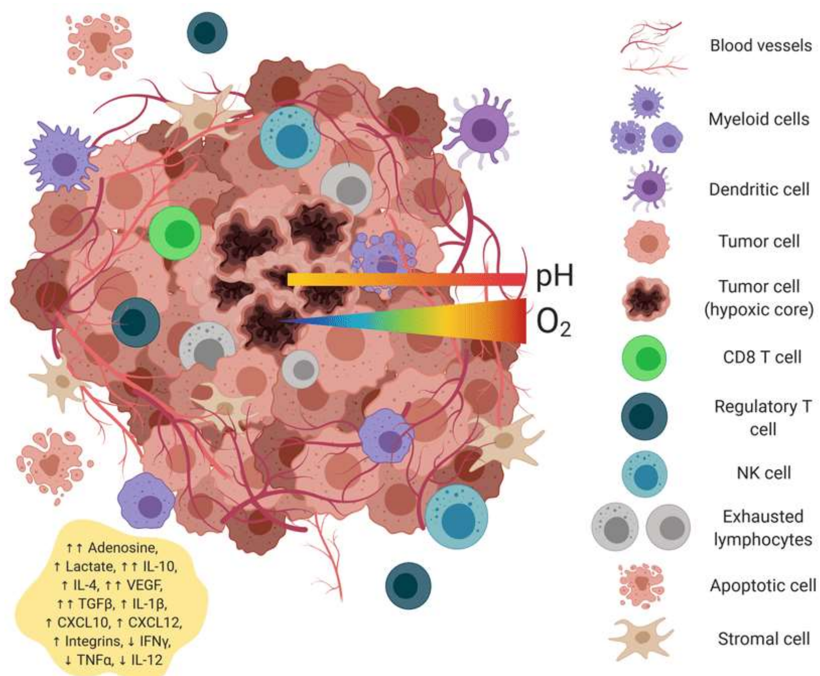
What is a Tumor Microenvironment (TME) ?

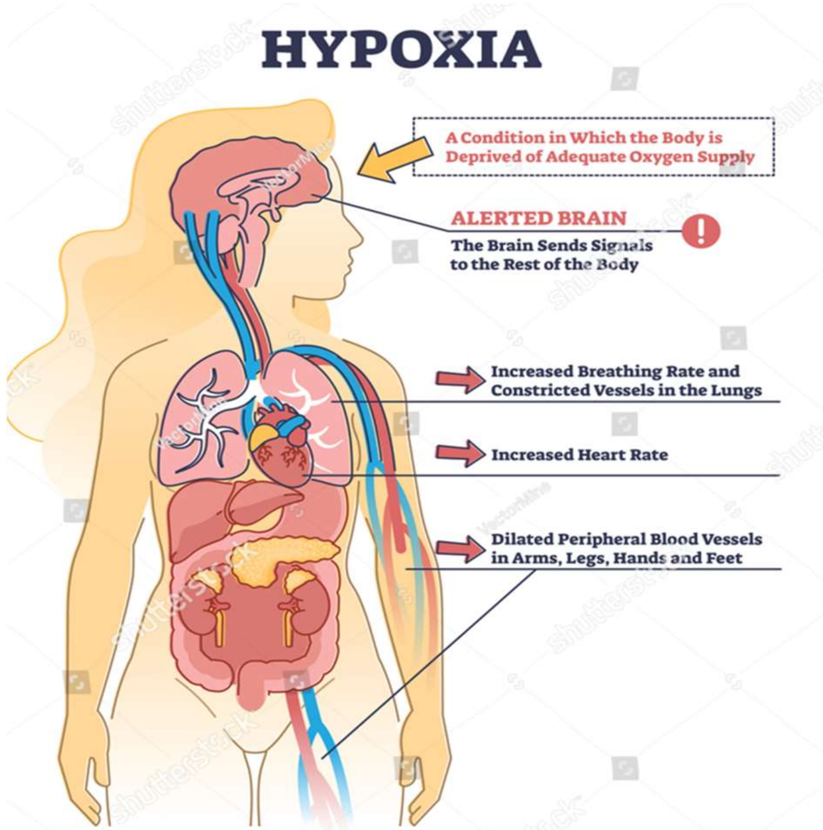
- Tumor: An abnormal mass of tissue that forms when cells grow and divide more than they should or do not die when they should
- TME: tumor microenvironment is the environment around a tumor
- Includes the surrounding blood vessels, immune cells, fibroblasts, signaling molecules and the extracellular matrix.
- The tumor and the TME are closely related and interact constantly.

A tumor and its TME



A tumor and its TME




HYPOXIA
A Condition in Which the Body is Deprived of Adequate Oxygen Supply
ALERTED BRAIN
The Brain Sends Signals to the Rest of the Body
Increased Breathing Rate and Constricted Vessels in the Lungs
Increased Heart Rate
Dilated Peripheral Blood Vessels in Arms, Legs, Hands and Feet

Tumor hypoxia = Lack of Oxygen in TME

- Hypoxia heterogeneity on radiotherapy and chemotherapy
- Decrease in Oxygen from tumor periphery to tumor center
- A larger radiation dose is needed for a tumor breakup
- Will enable successful follow-up chemotherapy
- We need a quantitative model that will guide the detailed dose

  needed for successful therapy

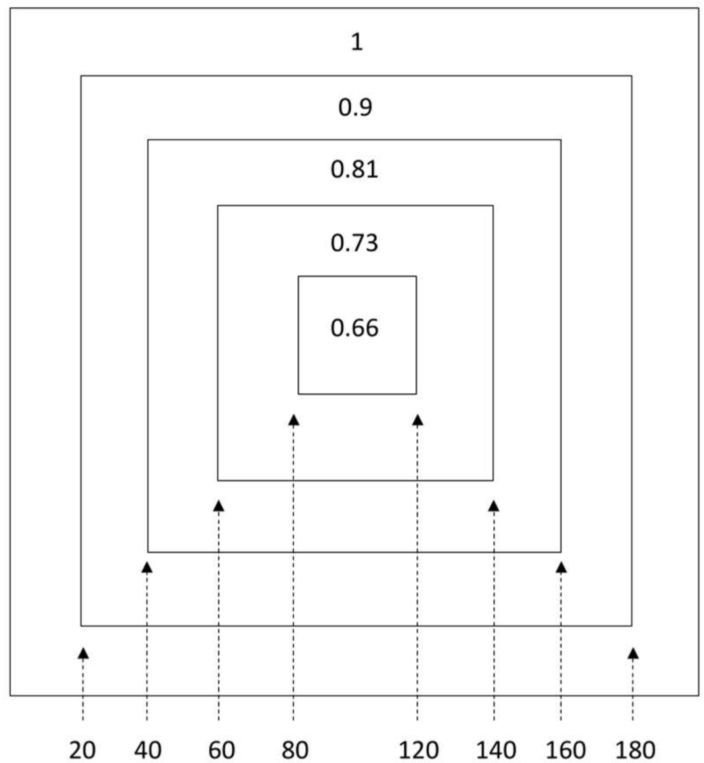
(1) Percolation lattice model
(2) Network model

- Simulate the tumor TME using these two geometrical models
- Network model better than lattice (brain is a network)
- Define a core (the tumor) in the middle of the system
- Split the area surrounding the core in different zones
- Vary the concentration of different species in the zones
- Use different probabilities to monitor the concentrations
- Observe how critical properties change as a function of the probabilities

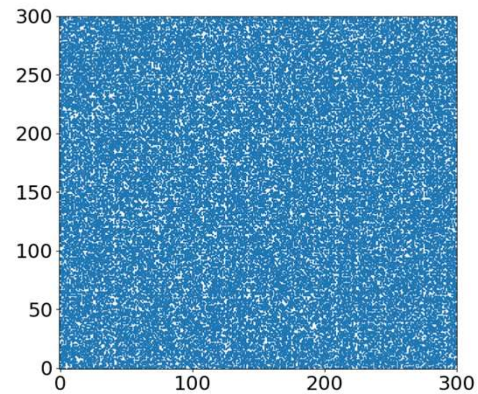
p = probability for removal of a node (site) (different p from previous notation)

- $p_i = (1-r)p_{i+1}$ probability of removal in successive zones i
- r= rate of reduction of the removal probability
- when r=large, means small probability for removal of a node
- when r=small, means large probability for removal,

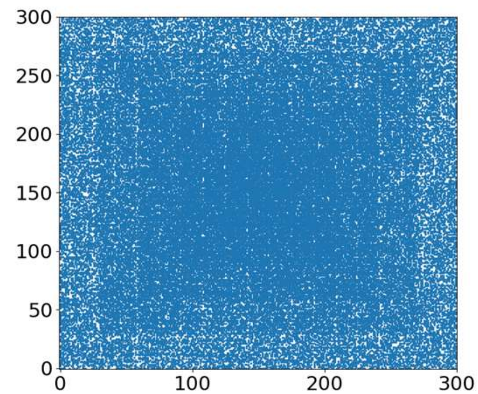
with r=0, being the maximum probability of removal

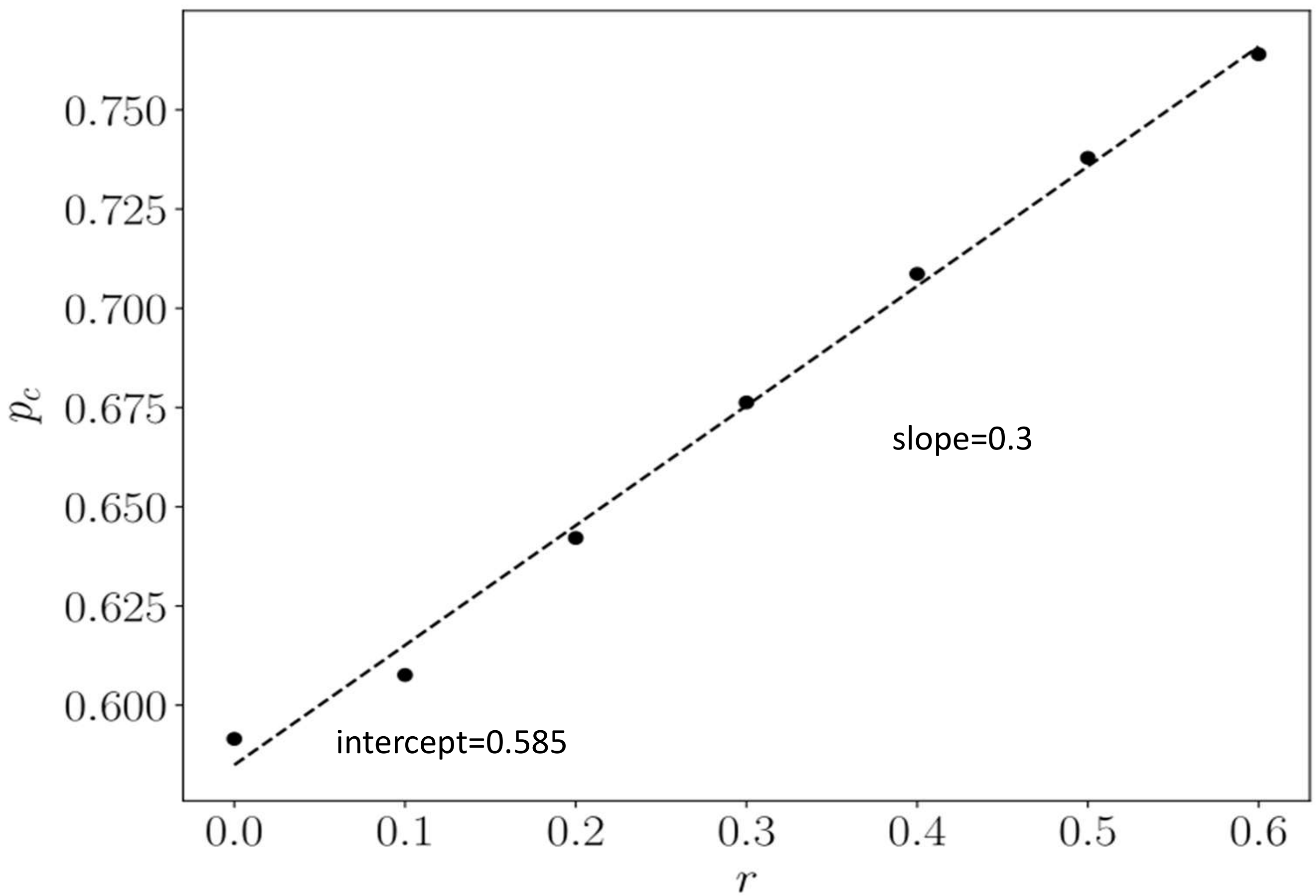

1
0.9
0.81
0.73
0.66
20
40
60
80
120
140
160
180

p=1



5 zones
r=0.4





0.750
0.725
0.700
0.675
0.650
0.625
0.600
p_c
slope=0.3
intercept=0.585
0.0
0.1
0.2
0.3
0.4
0.5
0.6
r

Summary - Conclusions

- Role of tumor hypoxia distribution in TME
- Acidosis (low pH), etc. may also be factors
- Will give information about the correct dose that will be needed in order to kill the tumor successfully
- Will lead to personalized medicine, since the TME is not the same in all patients, needing specialized treatment for each individual
- Will guide precision oncology

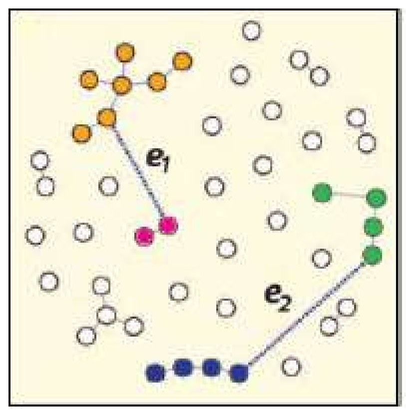
Summary-conlusions

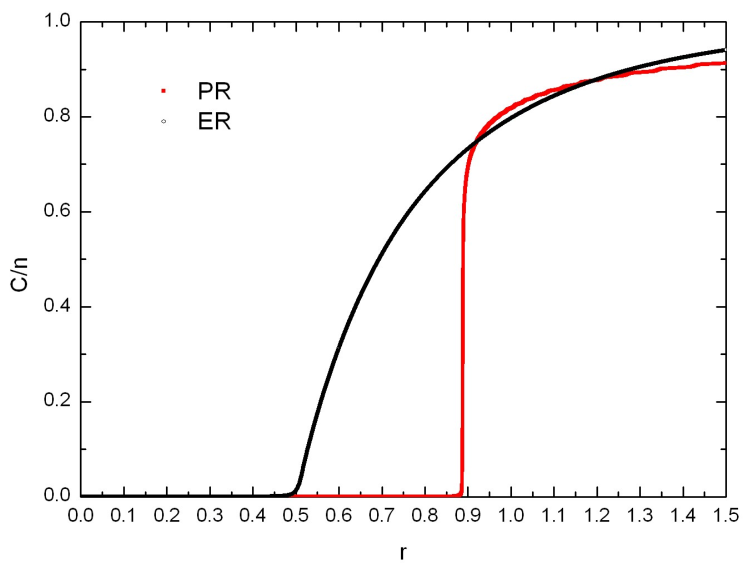
- Percolation is a very simple geometrical problem
- Has many applications in polymers, porous media, forest fires,

Achlioptas process

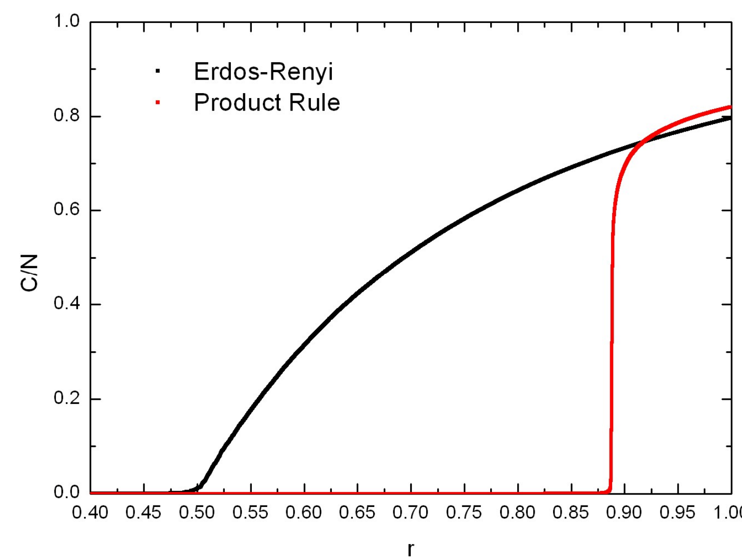
- developed in 2010
- new method of preparing the system
- use probe sites and fill lattice in such a way as to delay the criticality

Achlioptas process - product rule





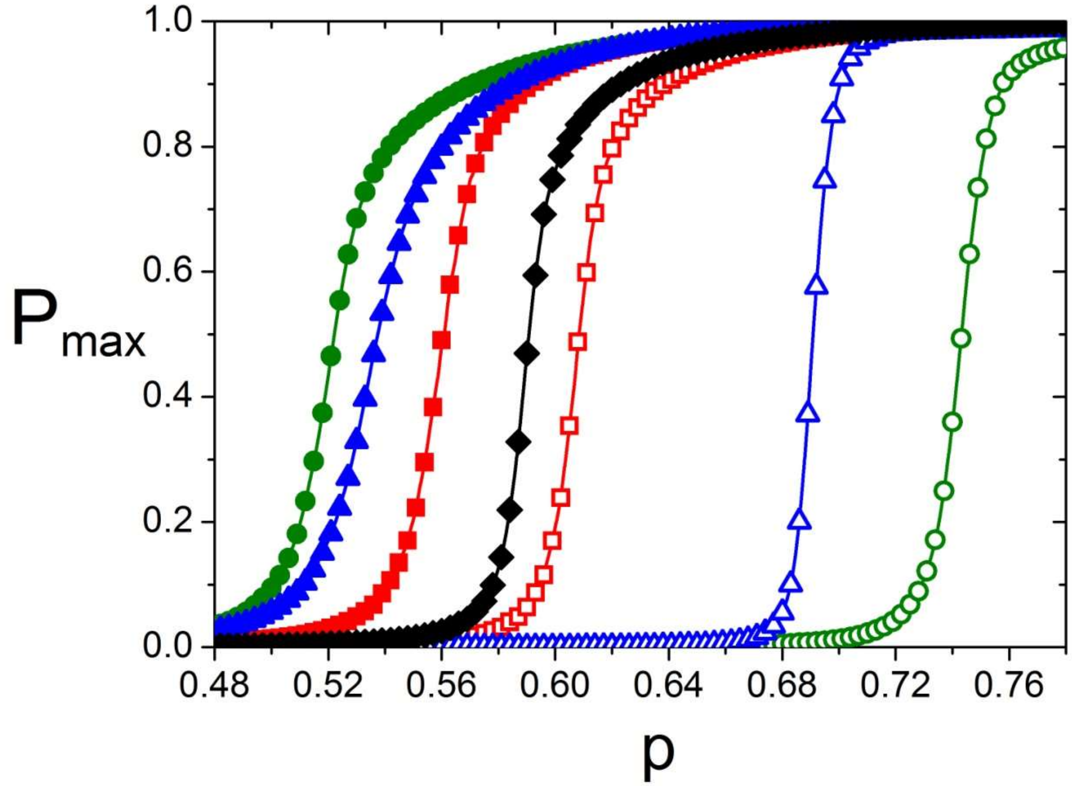
PR
ER
C/n
r
1.0
0.8
0.6
0.4
0.2
0.0
0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.1 1.2 1.3 1.4 1.5



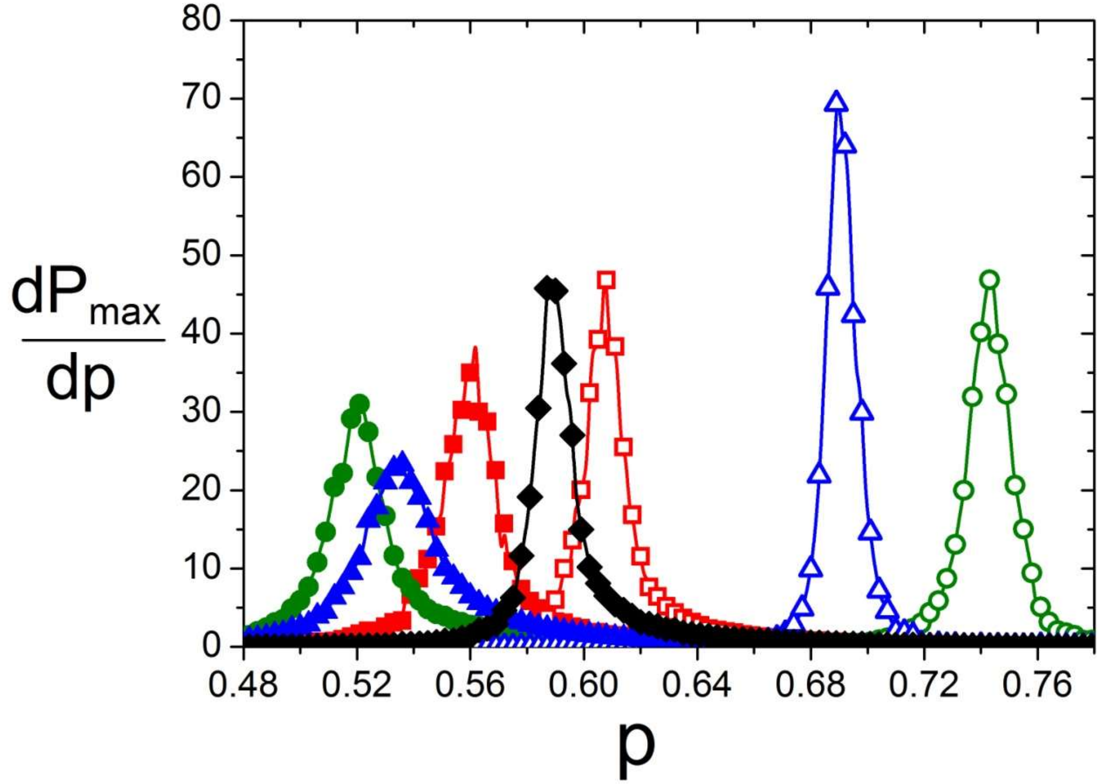
Erdos-Renyi
Product Rule
C/N
r
1.0
0.8
0.6
0.4
0.2
0.0
0.40 0.45 0.50 0.55 0.60 0.65 0.70 0.75 0.80 0.85 0.90 0.95 1.00

Many different variations

- Sum or product
- Allow the largest or the smallest
- Attraction or repulsion



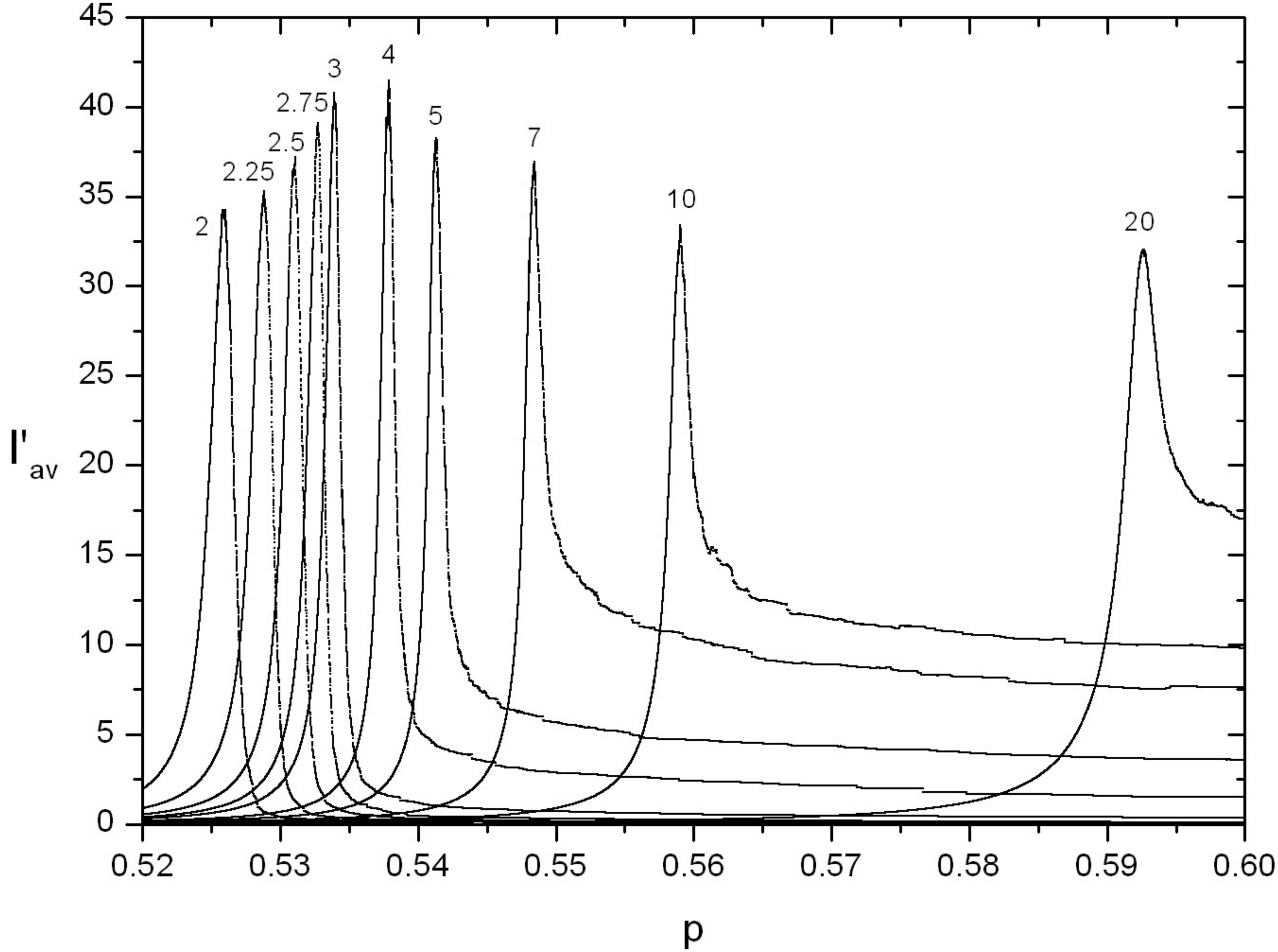
1.0
0.8
0.6
0.4
0.2
0.0
P_{max}
0.48
0.52
0.56
0.60
0.64
0.68
0.72
0.76
p



80
70
60
50
40
30
20
10
0
$\frac{dP_{max}}{dp}$
0.48
0.52
0.56
0.60
0.64
0.68
0.72
0.76
p

Critical percolation threshold values

Model	p_c	d_f
Classical percolation	0.5927	1.89 ± 0.02
Attraction model ($k = 1$)	0.5618	1.89 ± 0.03
Repulsion model ($k = 1$)	0.6100	1.88 ± 0.03
Product rule (delay)	0.7554	1.99 ± 0.01
Product rule (early emergence)	0.5315	1.87 ± 0.02
Sum rule (delay)	0.6942	1.99 ± 0.01
Sum rule (early emergence)	0.5433	1.88 ± 0.02



45
40
35
30
25
20
15
10
5
0
l'av
0.52
0.53
0.54
0.55
0.56
0.57
0.58
0.59
0.60
p
2
2.25
2.5
2.75
3
4
5
7
10
20

Summary: percolation

- Old problem
- Most useful paradigm in phase transitions
  (similar as Ising model)
- CMLT was first method, now many more
- Very useful in many-many different fields
- Problem is solved, but new variants emerge