Computer Simulation of Site Percolation on 2D Square Lattice and Its Application

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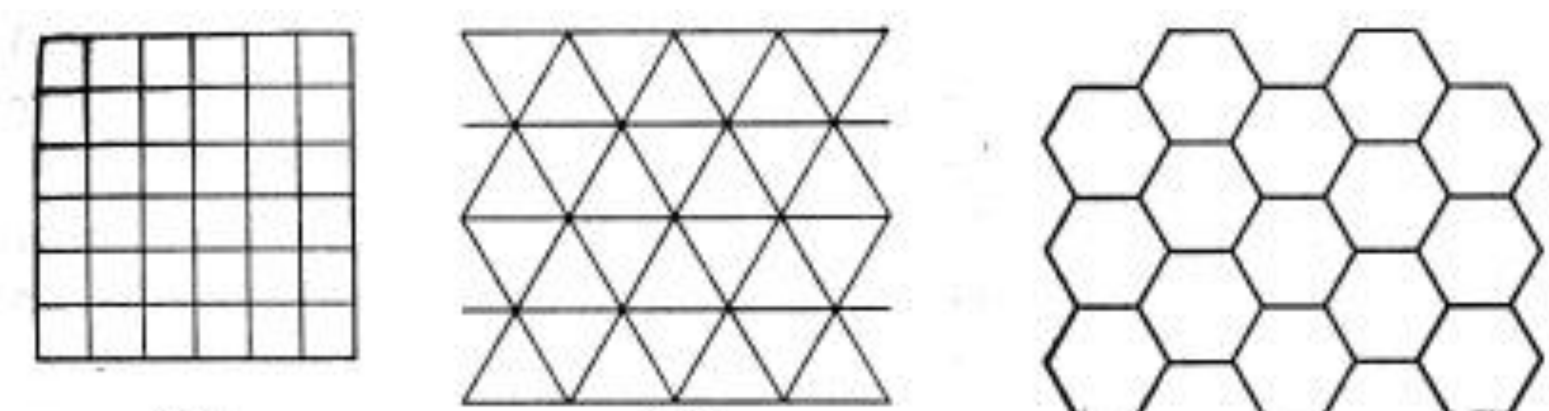
Preliminaries

1) Lattice and lattice types

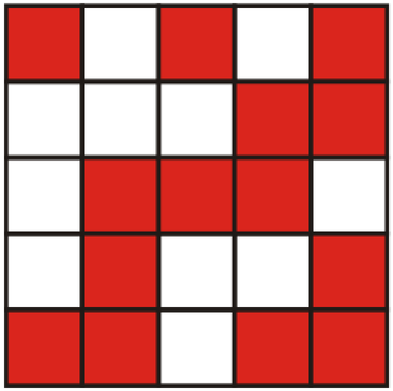
- Periodic arrangement of points (atoms) i.e. grid of 'Z^d' where 'Z' set of integers and 'd' is dimension
- Types of plane(d=2) lattice (a)Square ,(b)Triangular , (c) Honeycomb



(a) (b) (c)

2) Clusters

- Group of nearest neighbour which have same properties.
- No's of points (sites) in cluster is know as cluster size '*S*'.
- Number of cluster of size '*S*' is know as cluster no 'N_S'.
- Normalised cluster number is no's of cluster of size '*S*' per lattice site n_S.



In fig 1: n=5 and P=0.56 we have 2 cluster of size 1, 1 cluster of size 3 and 1 cluster of size 9.

What is Percolation?

- Simple probabilistic model to study lots of physics problem related to critical phenomena
- First introduced by *Broadbent and Hammersley* in 1957. While designing gas mask for use of coal mines.
- Its consist of lattice Z^d, in which each individual element is know as site
- Sites are occupied by probability P and empty with probability 1-P
- Group of occupied nearest neighbour is called as cluster
- When we found the cluster which connects opposite edges of lattice we say we found percolation for given occupying probability
- We consider the size of percolating cluster infinite since $n \longrightarrow \infty$

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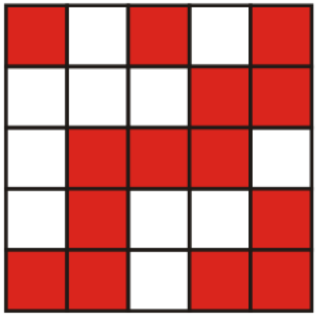
Types of Percolation

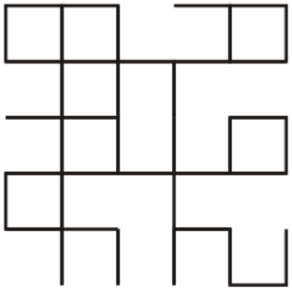
1)Site percolation

- Site percolation is defined as a grid of Z^d, with each site (vertex) to be occupied with probability P independently. Actually it is a graph of vertices where each vertex represent as a site. For d=2 it will look like fig .



2)Bond percolation

- Bond percolation is defined as a grid of Z^d, with each bond (edge) open or close with probability P independently. For d=2 it will look like fig



The Percolation Threshold p_c

- There is sudden change in system after certain value of occupying probability '*P*' such as
- If P_∞ is a probability of finding percolating cluster

$$P_\infty = 0 \qquad \text{if } P < PC$$
$$= 1 \qquad \text{if } P > PC$$

- So we have to find such value of occupying probability at which we observed the percolation in lattice 1st time. It is also know as critical probability

How to find p_c analytically?

- To find P_C we have to know average cluster size $\hat{S}$ *(P)* since it has a maximum value at $P=P_C$
- To calculate average cluster size $\hat{S}$, we have a to know W_S i.e. probability that any occupied site belong to a cluster of size *S*.

$$W_S(P) = \frac{S n_S}{\sum_S S\, n_S}$$

$$\hat{S}(P) = \sum_S S\, W_S$$

- Where n_S is number of *S* sized clusters per lattice site.

- To calculate n_S we suppose to know all lattice animals i.e. all cluster configuration for corresponding *S* size and perimeter *t.*

$$n_S(P) = \sum_t g_{St} P^S (1-P)^t$$

- where *S* is size of cluster and *t* is number of empty sites in edge of given cluster due to which it is of size *S*, g_{st} is no's of possible configuration of cluster for corresponding *S* and *t*, P is occupying probability.
- We can solve some special case using this methods such as 1D case where *t* has fixed value 2 and g_{s2} has fixed value for any *S* which is 1. from which we get that P_C=1 for 1D case

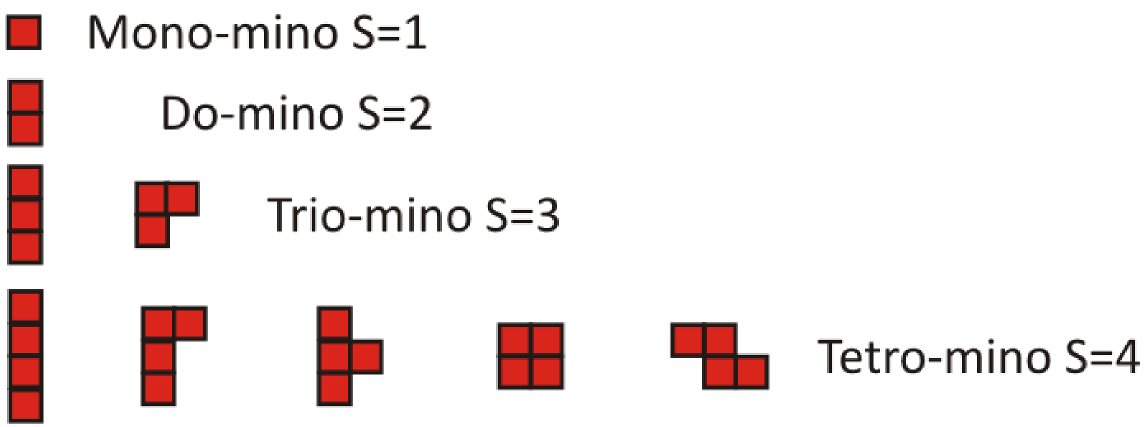
$$n_S(P) = P^S (1-P)^2$$

Problems to solve 2D case analytically

- We unable to solve this equation

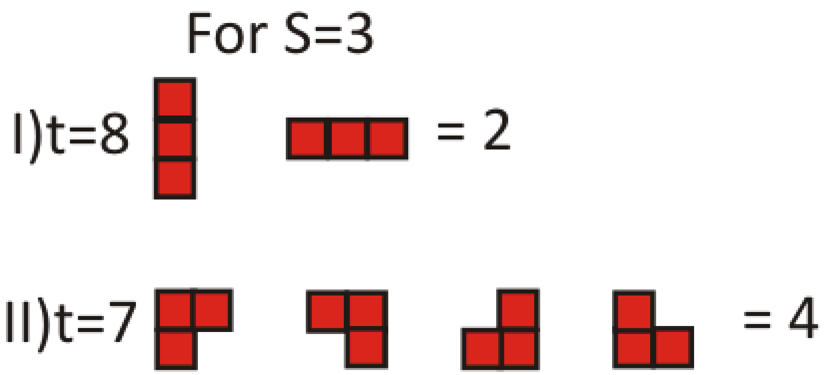
$$n_S(P) = \sum_t g_{St}\, P^S (1-P)^t$$

- Since we cant evaluate all values of g_{st} for corresponding *s* and *t*.



- In above image we shown some lattice animals for different *S* values to find P_C we have to know all lattice animals for *S* and *t*

- Take a simple case of *S=3* has two possible *t* vales 8,5 possible configurations will be as shown in below image.



g_{38}=2 and g_{37}=4 for simple case of size 3 has these values as S increased these no's will also vary large and it is really impossible! to calculate ns for any general value of s and t

- So to solve 2D case of site percolation we take help of computer simulation .

Algorithm to solve 2D site percolation problem

- To simulate this phenomena we used *Hoshen-Kopelmen* Algorithm.
- Theme of algorithm is that multiple Labelling technique.
- i.e. each individual cluster is represented by a unique label.
- In this algorithm the label clusters while occupying in my case I label each cluster after occupying.
- It has three simple steps

  1) Generate Empty Lattice,

  2) Occupy the Sites for Given Value of P,

  3)Re-Label Occupied Site

1) Generate Empty Lattice

By using array we generated a simple lattice we label each site of lattice by ‘o’ since lattice is empty.

2) Occupy the Sites for Given Value of P,

we start from any corner of lattice site, then we generate a pseudo random number if its less than occupying probability then we occupy that site by changing its label from 0 to 1.

We repeat same process for each site of lattice. The sites which are occupied we stores there co-ordinates since these sites are re-label as per clusters.

3)Re-Label Occupied Site

Now we have co-ordinates of all occupied sites i.e. all sites which have label 1. we go on each occupied sites check there label and re-label if require.

while re-label the sites we have 5 possibilities which are if (x , y) represents a sites for which we searching its nearest neighbour and (I , j) represents a its nearest neighbour then

i) (i, j) =1 and (x, y) =1

for this case we generate new label which is next integer after the previous label we used at vary 1st its 2

ii) (i, j)>1 and (x, y) =1 or vice versa

for this we re-label that site which has label 1 by its nearest neighbour

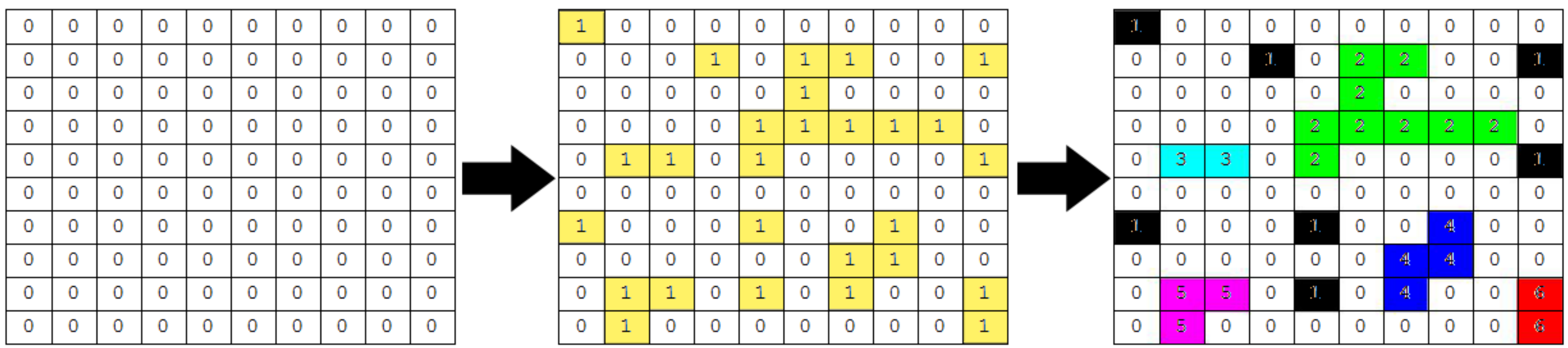
iii) (i, j)>1 and (x, y)>1 and (I ,j)<(x , y) vice versa

in this case we re-label the site which label is greater than the its neighbour simple illustration which represents algorithm and its steps

(A) Represents Empty Lattice

(B) Represents Occupy the Sites for Given Value of P

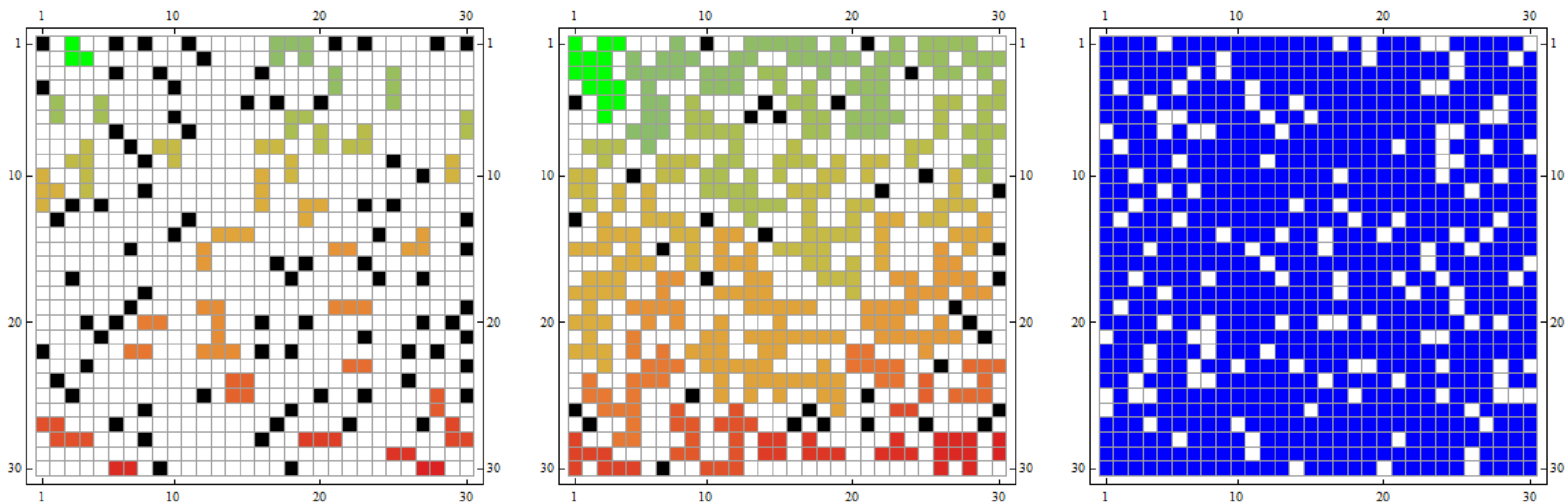
(C) Represents Re-Label Occupied Site



(A) (B) (C)

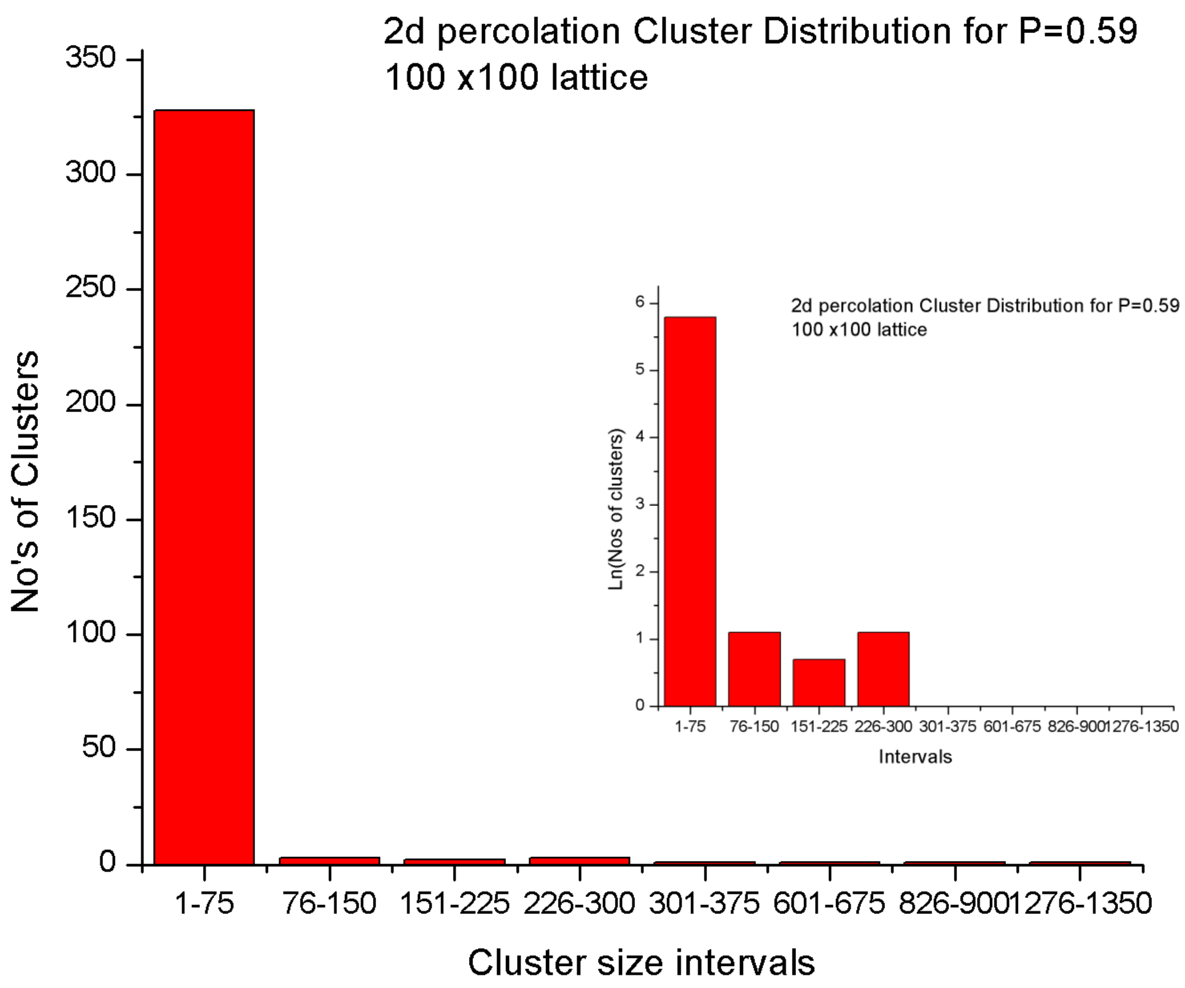
Results

1. Visualization of lattice for 30 x 30 three different P values

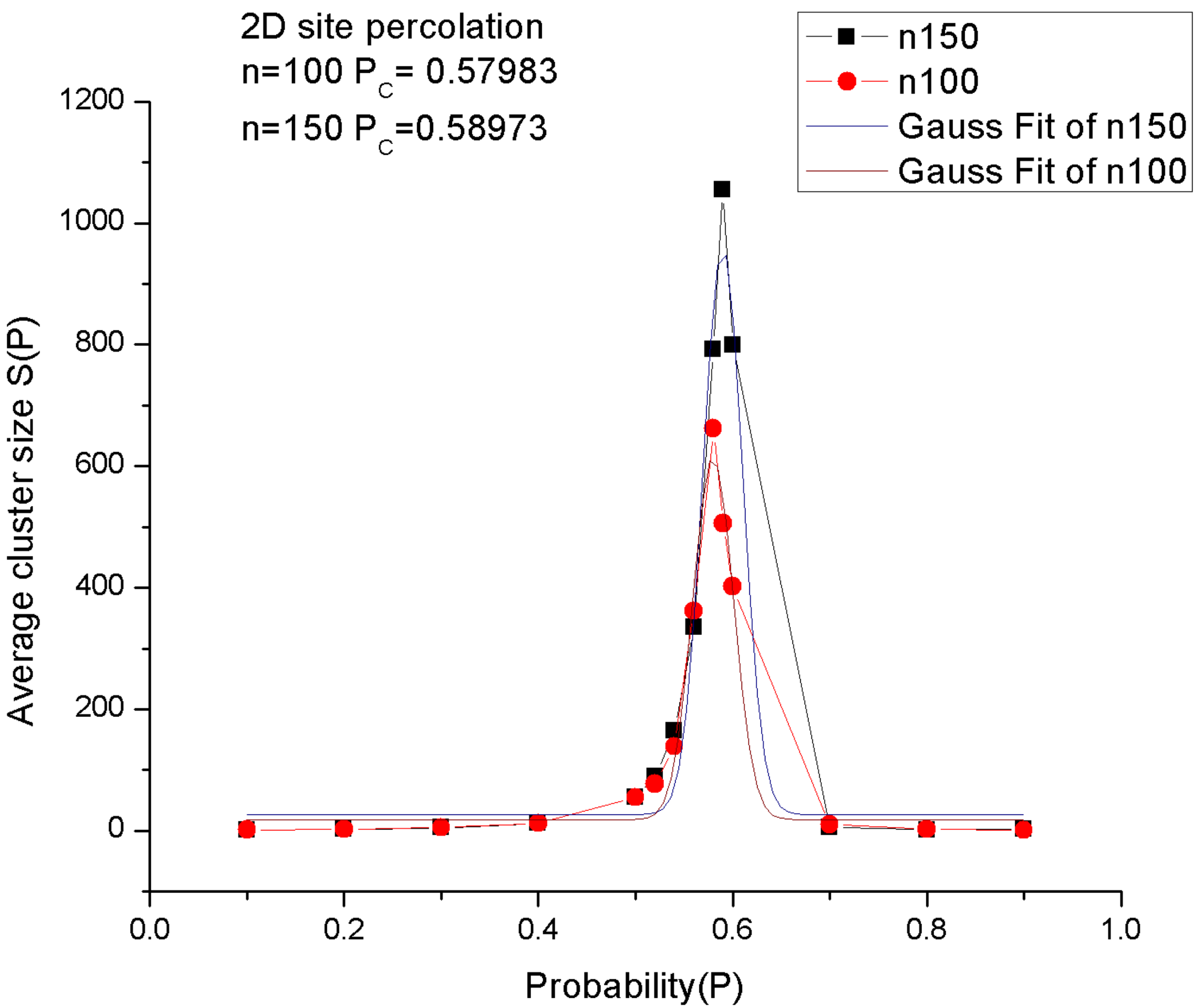


P=0.2 P=0.5 P=0.85

2. Cluster distribution for 100 x 100 P=0.59



2. Plot of average cluster size Vs occupying probability to find P_C

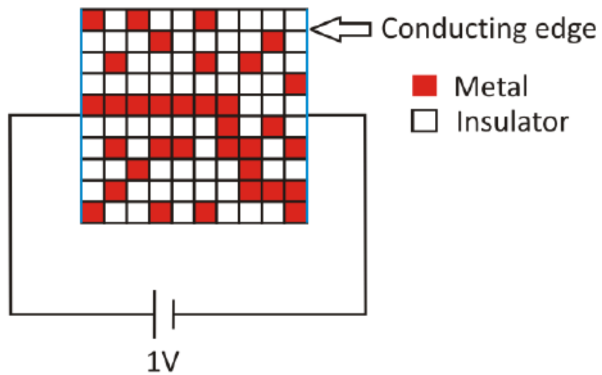


Percolation and Electrical Conductivity

Here we try to explain Insulator-Conductor transition using percolation by 1) Classical Experimental approach and 2)CAD approch

1) Classical Experimental approach (by **B.J. Last** and **D.J. Tohouless**)

They consider conducting sheet of graphite 127mm x 127mm drawn a grid of 50 x 50 so this converted a big sq sheet in to a large no's of small sq i.e. 2500 squares. They punching squares randomly such way it should overlap with its nearest neighbour.



now they measure resistance after every 1% of holes are punched(25 sites) using high sensitive instruments. The plot of resistivity Vs percentage of holes shows same behaviour as a plot of average cluster size Vs probability

Results of B.J. Last and D.J. Tohouless experiment

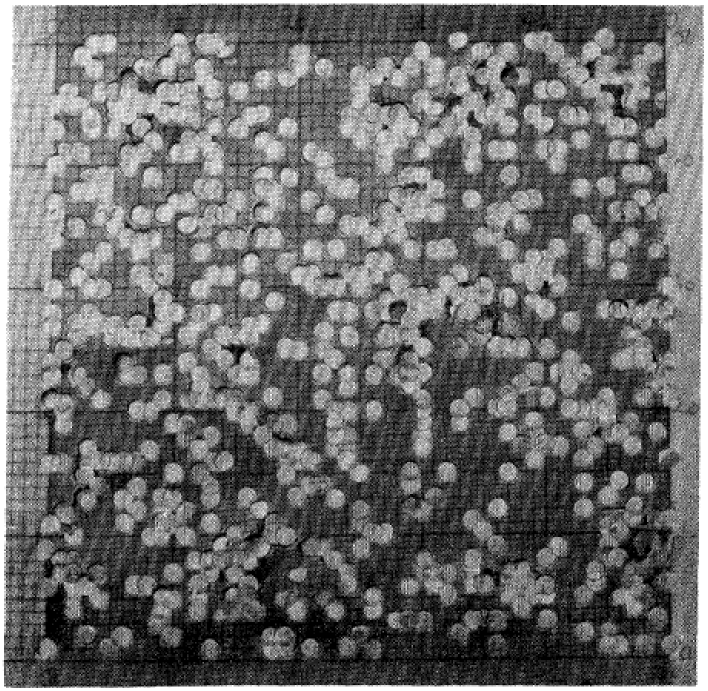
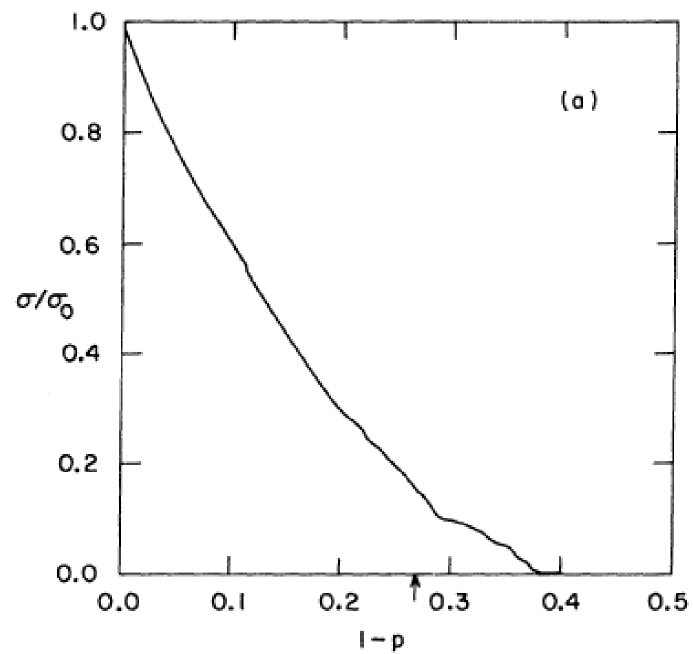


FIG. 1. Photograph of the sheet of conducting paper at the stage where the concentration of holes is 0.268.



2)CAD approch (**G.A. Schwartz** and **S.J. Luduena**)

they develop simple program which will produce simple particles of different size and shape. which are placated on 64 x 64 array. They print it using silver conducting ink. And measured a electrical resistance using some height sensitive device.

Results

Fig. 2. A picture of the layout with conducting particles for concentration $p = 0.35$. Some clusters begin to appear. The two lines on the right side are used to normalize the value of the resistance.

Thank You