COMPUTER SIMULATION OF SITE PERCOLATION ON 2D SQUARE LATTICE AND ITS APPLICATION

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By

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ABSTRACT

The Percolation Model is simple probabilistic tool to study lots of physics problems, which are related to critical Phenomena. Most interesting thing about percolation phenomena is that you don't have to know any rigorous mathematic to understand it, simple understanding of probability concept is more than sufficient to understand the phenomena. In present project I am trying to explain the concept of electrical conductivity in metal insulator transition by using the 2D site percolation model.

2D square lattice percolation problem is interesting since in any other lattice problems square lattice is simple example but here it is simple case for understanding the phenomena but to solve it analytically it really difficult or impossible! So we simulated this problem and try to solve it. To simulate it I used the *Hoshen-Kopelmen* algorithm [2]. the quantities in which we are interested to solve it are find cluster distribution for given occupation probability, from which we calculated average cluster size $\hat{S}$, using this we can calculate percolation threshold P_C and using concept percolation explain concept of electrical conductivity in metal insulator transition[5][6].

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LIST OF SYMBOLS

symbol	Meaning
n	order of lattice
$\boldsymbol{L}$	total number of sites
P	occupation probability
P_C	Percolation Threshold
S	cluster size i.e. total sites belongs to cluster
P_∞	Probability of percolation
S_∞	Size of percolating cluster
$\hat{S}$	Average cluster size
N_S	Numbers of clusters of size S
n_S	Numbers of S sized clusters per lattice site
t	Perimeters , the numbers of empty lattice sites in neighbor of borders sites of cluster
g_{St}	The numbers of lattice animals (cluster configuration) with size S and perimeter t
W_S	Probability that any site belongs to cluster S
d	Dimension of lattice
σ	Conductivity
μ	Critical exponent
$\boldsymbol{Z}$	Set of Integers

INTRODUCTION

1) PERCOLATION

Percolation theory was introduced by *Broadbent* and *Hammersley* in 1957[1]. While designing gas mask for use of coal mines. *Broadbent* came across an interesting problem regarding motion of gas in carbon granules which has pores that are connected together in an intricate manner to form a complicated maze due to which gas get filtered. He presented this problem to mathematician *Hammersley* then they called this phenomenon as a percolation.

In order to explain percolation consider a square wooden strip, with small thickness which will look like *fig 1(A)* .Now draw a square grid on it , so it will look like a square lattice *fig 1(B)* . A single big square is divided into many small squares. Each small square we called as site. Number of sites in a single row or column is called size of lattice *n.* so the total sites will be ***L=****n x n.* Now we want to drill sites randomly and independently. If the site is drilled then we called such site as occupied site otherwise empty. We occupy sites with occupation probability *P* so *1-P will* be the probability that site is empty. After occupying which will look like *fig 1(C)* in which colored sites represented an occupied sites and white site represented an empty sites.

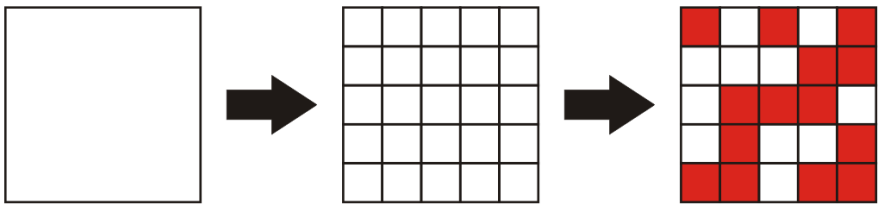

Figure 1

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. It is the percolating cluster so we consider its size is infinite. To find cluster distribution we define a cluster number N_S *as a numbers of cluster of size S. for fig 1.1 (C)* $N_1=2$, $N_3=1$, $N_9=1$

Now we started connecting the nearest-neighbor of occupied site if they are occupied. Nearest-neighbor is simply number of sites which are at same distance from site for which we searching nearest-neighbor. For present case i.e. for 2D square lattice it's four which are up, down, left and right. After connecting this, we will have a group of occupied site which are nearest-neighbor of each other, such a group we called as a cluster. Number of sites in a cluster is called as a size of cluster *S*. Minimum size of cluster is *1*, an isolated occupied site.

In clusters if we found a cluster which able to established the connection between 1^{st} row and n^{th} row or 1^{st} column and n^{th} column or both then we say that we found percolating cluster or simply we say we found percolation for given value of occupational probability P. For finite size of lattice n a size of a percolating cluster S_∞ is finite. It is due to finiteness of n, this cluster may grow to infinity it stopped growing since our n is finite and since we working in limit of $n \longrightarrow \infty$ so $S_\infty \longrightarrow \infty$. So for all values of n we consider size of percolating cluster as infinite $S_\infty = \infty$.

2) TYPES OF PERCOLATION

There are two important types of percolation 'site percolation' and 'bond percolation'.

I) BOND PERCOLATION

Bond percolation is defined as a grid of $\mathbf{Z^d}$, with each bond (edge) open or close with probability P independently. Where Z is a set of all integers and d is the dimension of grid. For d=2 it will look like *fig 2.*

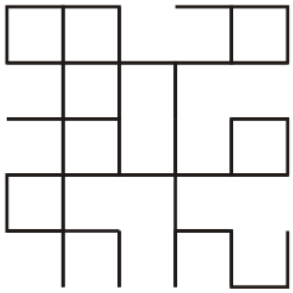

Figure 2

II) SITE PERCOLATION:

Site percolation is defined as a grid of $\mathbf{Z^d}$, 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 as shown in *fig 1.1* for d=2.

Site percolation is generalization of bond percolation, every bond percolation can be represented by site percolation but not other way around, percolation is simply group or cluster of infinite connected sites or bonds, since we consider that percolating cluster has a infinite size, and percolation threshold for site percolation is always larger that bond percolation. And nearest neighbor for 2D square lattice site percolation is 4 for bond it is 6.

3) THE CRITICAL PROBABILITY P_C (PERCOLATION THRESHOLD)

We are interested to find critical value of occupational probability P_C at which we found percolation first time, it is also known as percolation threshold. If occupational probability is less than percolation threshold then there is no percolation and if it is greater than percolation threshold then there is always we observed percolation.

Let P_∞ is a probability of percolation.

For infinite size i.e. $n=\infty$

$$P_\infty = 0 \quad \text{if } P < P_C \qquad \ldots (1)$$
$$= 1 \quad \text{if } P > P_C$$

For finite size i.e. $n=$ *finite*

$$P_\infty = 0 \quad \text{if } P < P_C \qquad \ldots (2)$$
$$> 0 \quad \text{if } P > P_C$$

1D SITE PERCOLATION

1D case is very simple and analytically solvable. Many of the characteristics features are seen in 1D case also, and it is very helpful to understand the concept of percolation.

Imagine a 1D lattice with an infinite number of sites (small squares) of equal size arranged in line. Each site has probability *P* of being occupied, consequently *1-P* of being empty these are two states which are only possible. This will look like fig 3.

Figure 3

In fig 3 white sites are empty sites and red sites are occupied sites. in a part of infinite 1d lattice shown above, there are 2 cluster of size 1, 1 cluster of size 2, 1 cluster of size 3 i.e. $N_1=2$, $N_2=1$, $N_3=1$

To solve this problem analytically we have series method which like this,

$$n_S(P) = \sum_t g_{St}\, P^S (1-P)^t \qquad \dots (3)$$

Where n_S is number of *S* sized clusters per lattice site. to calculate n_S we have to know all cluster size configuration which are known as lattice animals(more idea will clear in next chapter), any cluster will be of size *S* since *S* numbers of sites are occupied if *P* is probability of occupancy then P^S will be probability of *S* sites are occupied and any cluster is size *S* since its edge neighbors are empty, we represented all numbers of empty sites are at the edge of cluster of size *S* by *t* then these sites are empty by probability $(1-P)^t$. For each value of *S* and *t* we will have different cluster configurations. For each S we will have different *t* values, by summing over all t values we can calculate n_s.

This will be useful to calculate an average cluster size from which we can find 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*. which is define as.

$$W_S(P) = \frac{S n_S}{\sum_S S\, n_S} \qquad \dots (4)$$

$$\sum_S S\, n_S(P) = P \quad if\ P < P_C \qquad \dots (5)$$

Sum over all values of S into W_S we can calculate average cluster size $\hat{S}$, for calculating we neglected percolating cluster since they have infinite size i.e. $S_\infty=\infty$, so average cluster size will be

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

$$\hat{S}(P) = \sum_S S \frac{S n_s}{\sum_S S\, n_s} \qquad \ldots (6)$$

For 1D case,

$t=2$ i.e. cluster is of size S because of the site before 1st site of cluster and site after last site of cluster are empty. $g_{st}=1$ i.e. for any value of S there is only one possible configuration since t is fixed.

$$n_S(P) = P^S(1-P)^2 \qquad \ldots (7)$$

After simplifying *(7)* we get

$$n_S(P) = \frac{SN_S}{L} \qquad \ldots (8)$$

Were, L= total site for 1D $n=L$ We know that average cluster size is blows at P_C so by using all these quantities we can find P_C for 1D percolation problem. Some results of 1d percolation which I produced using computer simulation.

1D RESULTS

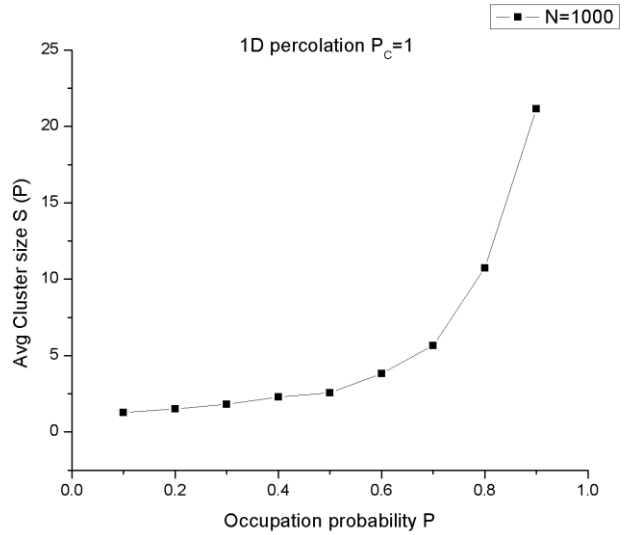

Figure 4

in fig 4 we plotted graph of average cluster size Vs occupation probability which shoots at P=PC so here P_C=1 for each value of P we calculated average cluster size 10 times then taken average of it so P_C is averaged value.

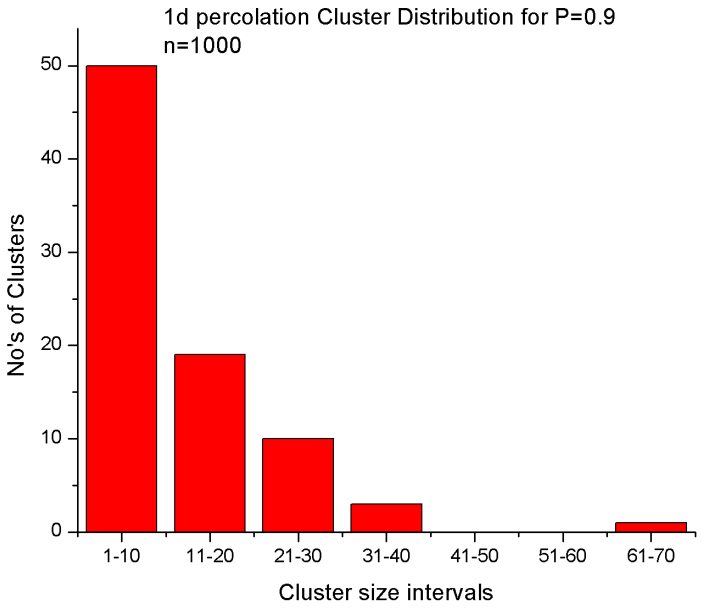

Figure 5

in fig 5 we shown cluster distribution at p=0.9

2D SITE PERCOLATION

The percolation problem for 1D is solved analytically, but for 2D is really hard or impossible to solve it analytically! Why? Answer will be discussed in this section.

To solve this problem, we have to solve eq. *(3)* for all values of perimeter *t* and cluster size *S.* for 1D perimeter has single value i.e. *2* but for 2D it will have infinite value or it's a function of *n* i.e. size of lattice. To find perimeter we have to know *animals* of given lattice for corresponding cluster sizes.

Animals of lattice are nothing but the cluster configuration for corresponding size of cluster and perimeter. More idea regarding animals will be clear in *fig 6*.

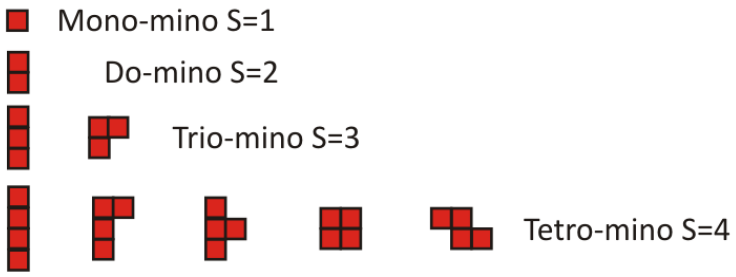

Figure 6

In fig 6 we show possible animals for corresponding S values i.e. for S=1,t=4 has 1, S=2,t=6 has 2, s=3,t=5,7 has 2+4=6, s=4,t=10,8,6,8,6 has 2+8+4+1+4=19 possible cluster configurations this will give a value of g_{st}.

Please note that we have these values for corresponding cluster configurations since we are considered lattice symmetries such as rotational, reflection etc. more idea of symmetry will clear in *fig 7*

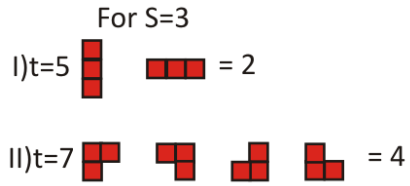

Figure 7

In fig 7 we can see all possible cluster configuration for s=3. First animal has two possible configurations by rotating same configuration to 90^0 *in clock wise sense. same way for second animal have four possible configuration by rotating four times by* 90^0 *in clock wise sense* $g_{35} = 2$, $g_{37} = 4$

For 2D case, it is really difficult to sum over all possible perimeter *t.* so there seems to be no exact solution for any value of *t* and *S* available at present. So we take help of computer simulation to solve it.

ALGORITHM

Hoshen-Kopelmen algorithm [2] is simple algorithm with theme that each individual cluster supposes to have a unique label, which also known as multiple is labeling technique. Original algorithm is that give unique label to site while occupying. But I modified little bit to make it simple for me.

It has three simple steps which are first generate a lattice and fill it with zero as zero label represent an empty site which will look like *fig 7(A)*. Now occupy the sites randomly and independently by changing label from zero to one as one label represent an occupied site which will look like *fig 7(B)*. Now we re-label all occupied sites as per which site belongs to which cluster which will look like *fig 7(C)*.

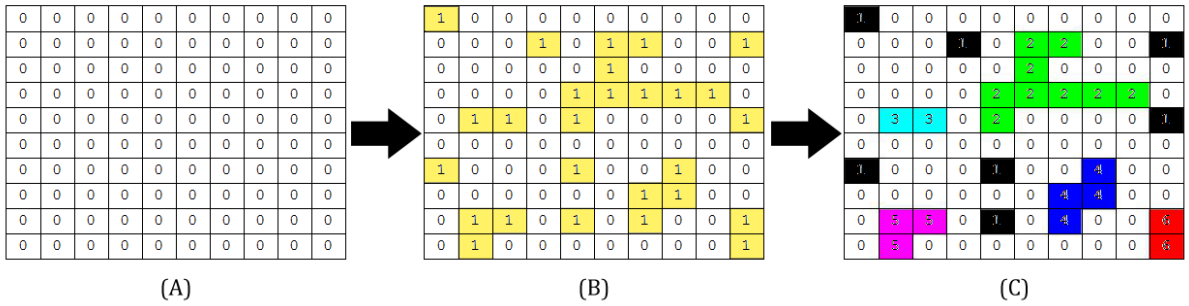

Figure 8

In fig 7 n=10, (A) represents an empty lattice, (B) represents an occupied for P=0.3 where, (C) after re-labeling as per clusters. where we have N_1=7,N_2=2,N_3=1,N_4=1,N_9=1.

I) GENERATING EMPTY LATTICE

To generate an empty lattice we used 2D array and allocated it to input value of *n* i.e. size of lattice. Since we are simulating a 2D site percolation. As per our convention for empty site is zero labelled.

II) OCCUPYING FOR GIVEN PROBABILITY

The site occupation is carried out as follows. First we choose a one of the corner site of lattice to stat. then we called a random number say r, if r is less than occupation probability p then we occupy that site by changing its label then we proceeds to next site continue for all rows.

While occupying site we storing each sites co-ordinates in separate arrays which are occupied, i.e. row position in $\boldsymbol{R_n}$ and column positions in $\boldsymbol{C_n}$. since we want to re-label all occupied sites. We do this for each site of lattice for each site should be equal probable.

For pseudo-random number generator I used an inbuilt random number generator of FORTRAN compiler. For randomness I am changing its seed for every execution. Seed is simply input for any random generator.

III) RE-LABELLING

As I mention us storing co-ordinates of each occupied sites, now we will use them to re-label it for identifying clusters. I will explain it using above example for which we are having a sequence of row and column which represent an occupied sites, as below.

No	R_n	C_n
1	1	1
2	2	4
3	2	6
4	2	7
5	2	10
. . .	. . .	. . .
27	10	10

First for each pair of **Rn, Cn** we check it's all nearest neighbour are exist in these array itself. For this case for first entry i.e. (1, 1) possible neighbours are (2, 1) and (1, 2) which are not belongs to these arrays so we will not change its label. Since we reserved label *1* for cluster of size of *1.* For second site also no nearest neighbour found, so we will keep its label. but for third point i.e. (2, 6) we found one neighbour which belongs to this array which is (2, 7), now we check both the sites i.e. what label they have, then there are three possibilities we represented a site for which we searching its nearest neighbour, we represented it by (i, j) and site which found nearest neighbour of it, is represented by (x, y) which are as follows;

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

for this possibility, we generate new label ,since we reserved 1 for isolated clusters and these two's sites are nearest neighbour of each other still have label one. So new label will be next integer of previous cluster label for this case it is 2, so both sites will labelled as 2.

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

if two sites are nearest neighbour of each other and one of them has label greater than one and another has one then we put the label which is large at site which has label one. For this case we label (2, 7) = (2, 6) and vice versa for opposite case.

iii) (i, j)>1 and (x, y)>1

this case has two sub cases which are as below; if (2, 6)<(2, 7) for this case we change the label of site which label by large integer to site which is labelled by small integer, for this it will be (2,7)=(2,6) vice versa for opposite case.

After doing these steps until each cluster has unique label. Then we will have cluster distribution, for each label we know the size of cluster from which we can find

N_S i.e. numbers of clusters of size S which will be helpful to calculate the average cluster size to find P_C percolation threshold. For above case we will have this table as bellow;

Label	Cluster size(S)	N_S
1	1	7
2	9	1
3	2	2
4	4	1
5	3	1
6	2	2

There is one small difference between my logic and original *Hoshen-Kopelmen* logic which is; in H-K they use multiples labels while occupying sites, while I use it after occupying the sites. And results which I found are perfectly matching which the available results [3].

2D RESULTS

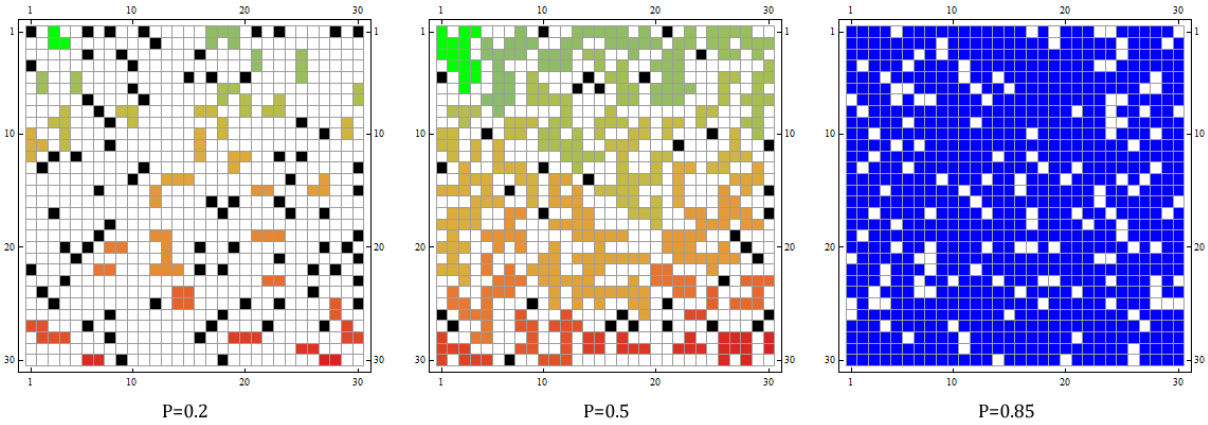

Figure 9

In figs 9 some plots of 30 x 30 lattices for different P values.

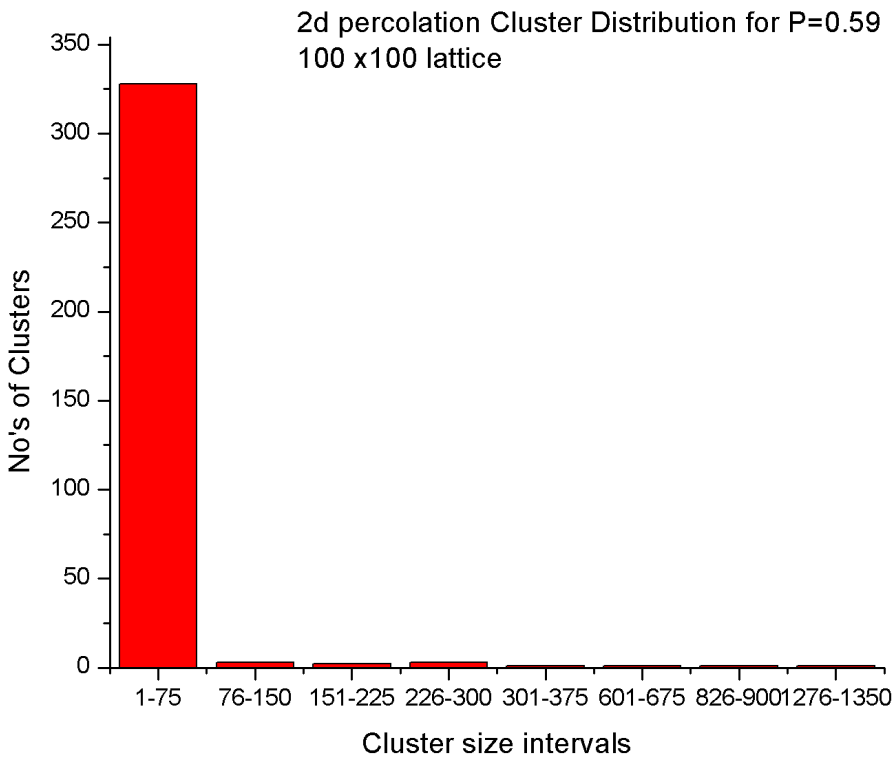

Figure 10

In fig 10 cluster distribution of 100 x 100 for p=0.59 we can observed sharp decrease in distribution since P= P_C approximately

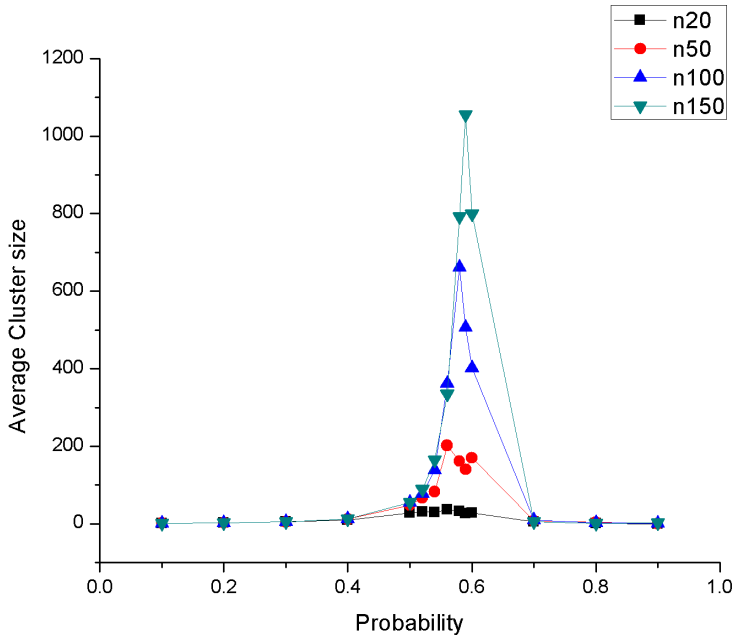

Figure 11

In fig 11 for each probability evaluated $\hat{S}$ for ten different seed then taken average of it. As we increase n peak becomes sharper and sharper at $P=P_C$

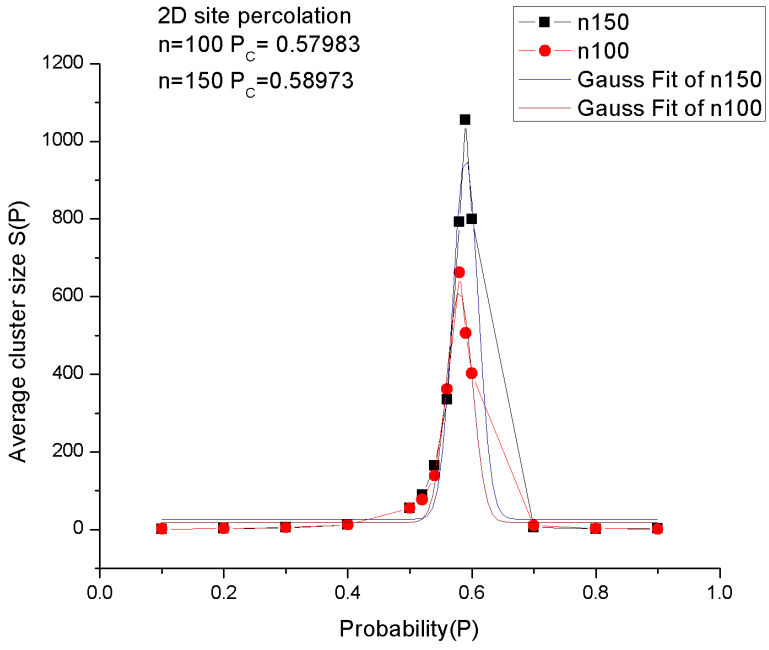

Figure 12

In fig 12 we done Gaussian fitting for n=100 and 150 from which we calculated P_C from we observed that for small value of n PC has large error as n increased error becomes small and small.

ELECTRICAL CONDUCTIVITY AND PERCOLATION

One of the interesting percolation related problem to study is electrical behavior of a system of conducting particles dispersed in insulating matrix. These disordered conductor-insulator composites show a variety of incompletely understood phenomena. The electrical behavior of this system can be described by simple percolation model in which conducting sites are distributed randomly on insulating medium. When the concentration of conducting sites is lower than the critical concentration or percolation threshold P_C then there is no macroscopic conductivity pathway exists. And the composite remains in insulating phase. When the concentration exceeds the critical value. The system becomes electrically conducting.

$$\sigma = \begin{cases} 0 & if\ P < P_C \\ \sigma_0 (P - P_C)^{\mu} & if\ P > P_C \end{cases} \quad \dots (9)$$

Where P is a concentration of conducting sites and P_C is percolation threshold. The power law behavior of conductivity is as shown in eq. *(9)* is expected to hold in vicinity of P_C actually near and above P_C. Where μ is critical exponent which only depends on dimension of system not on its small scale details. This we called the universality which means that it is same for different lattice geometry and even continuum system.

another simple way to understand the concept of conductivity by percolations points of perspective let consider square lattice of insulating material when site is occupied means the insulator site is replace by metal site, an electrical d.c. current can flow only through the metal sites if a unit voltage is applied between sides of lattice as shown in fig 12.

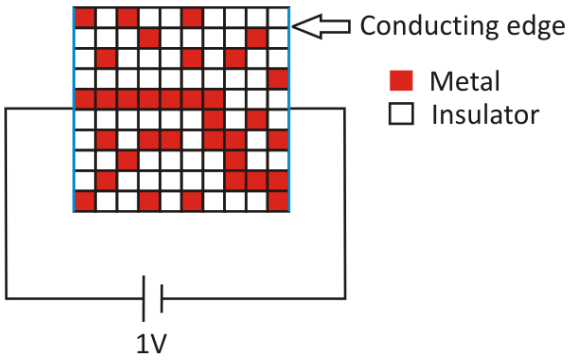

Figure 13

in fig 13 we represented colored site as metal and empty site as insulator we randomly replacing empty (i.e. insulator) sites by metal sites for corresponding P value initially no current will flow from the circuit due to all sites are empty at certain value of occupied site the suddenly current start flowing from circuit, since whole lattice is placed in two conducting plates.

Although the idea of percolation transition is conceptually simple, few analytic solutions are also available for special cases. Moreover is difficult to determine these

parameters for real system as conducting particles in insulating matrix. There are lots of attempts to solve this problem. But of every approach has different μ values for experimental approach were obtain from *Watson* and *Leath* [4] t=1.38±0.12 exact value of t=1.1±0.3 for 2D case. Modern experimental approach was by *Gustavo* and *Silvio* in 2003[5] which will be explain in next section.

1) CLASSICAL EXPERIMENTAL APPROACH

One of the simplest approaches to find conductivity exponent t was established by experiment done by *Last* and *Thouless* in 1971[6]. they taken a thin sheet of graphite of dimension 5 in x 5 in (127mm x 127mm) covered by square grid of spacing 0.1 in (2.54mm). So the continuum sheet converted to discrete grid of 2500 sites each of which may be open or closed. A hole punched site will be closed. Hole having a size of 4mm in diameter and thus first and second nearest-neighbors overlap. The reason for making holes size larger than site was to avoid problems due to two nearest-neighbor holes are not completely blocking off the bond between them.

The holes were punched randomly in paper with the aid of table of random numbers to determine co-ordinates. The resistance was measured after 25 sites are closed (i.e. approximately every 1% holes, allowing for repeated pairs). For measurement high-accuracy and high-in-put-impedance digital voltmeter were used. The results observed in this experiment are conductance becomes zero after a certain concentration of holes i.e. near 0.4 it is concentration of close sites so the concentration of open cites will be 0.6.

2) CAD EXPERIMENTAL APPROACH

This most recent and advanced approach to study two dimensional percolations using Compute Aid Design by *Gustavo* and *Sivilo* [5]. They develop program to draw a small black particles over a white background particles are placed with probability *P* on 64 x 64 lattices. This program has graphical interface from which we can change the shape of particles and lattice geometry. When the layout is ready then it is printed on *Hewlett Packard 692C* ink jet printer with silver conducting ink. We can measure electrical resistance directly using *Hewlett Packard 34401A* multimeter.

To avoid problem arising from variation of ink level or paper type, program draw a two continuous lines near layout. So first resistance of these two lines is measured and averaged. Then the resistance of layout is normalized by dividing it by this average. Although the resistance of layout is depends on the ink level, paper type, and room condition. The normalized resistance value is all most constant for each layout. With an error less than 3% independent of above conditions. The contact resistance between silver paint and ink is negligible compare to resistance of layout and it was not taken in to account in the analysis.

CONCLUSION

In present report we conceptually understood percolation phenomena. How to approch percolation problem , is clearly understood by solving 1D percolation problem analytically. We discussed two simple types of percolation i.e. site and bond. We also discussed why we are not able to analytically solve 2D square lattice site percolation problem.

So one tried to solve 2D square lattice percolation problem by simulating it using *Hoshen* and *Kopelman* algorithm. We found P_C for n=150 is 0.58973 which is approximately equal to0.59 and is matching with the available results, we observed that as we increase *n* the peak becomes sharper and sharper. As we move towards P_C there is sharp decrease in cluster distribution. Along with that we produced visualization of this simulation using Mathematica 8(i.e. matrix plot). We discussed the simple physical problem of metal insulator transition by using percolation perspective, also different experimental technique to solve this problem has been explored.

ACKNOWLEDGEMENTS

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