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A COMPUTER MATHEMATICAL MODEL OF A PERCOLATION GRID

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We propose a mathematical model of two- and three-dimensional percolation grids, on the basis of which we determine certain critical indices and the fractal dimensionality of an infinite cluster.

INTRODUCTION

Recently, in the description of the structure of various micrononuniform systems and their properties intensive use has been made of various percolation models [1-3]. In most of the cases, percolation models are produced by means of finite grids whose dimensions are limited by the memory volume of the computer. Results obtained in such grids must be extrapolated to grids of infinite size and serve as the basis from which to ascertain the qualitative behavior in the properties of percolation systems. In the following we describe a mathematical model which exhibits a fractal asymptote and which allows us to calculate the precise values of the critical indices and properties of percolation systems.

In these grid models we distinguish between linkage and node problems. In the linkage (node) problem we study the properties of the grid on a change in the concentration of whole linkages (nodes) v from 1-0.

The critical concentration v_c at which an infinite cluster (IC) arises is referred to as the penetration threshold and for the linkage problem this is denoted as $v_{c,s}^{(d)}$, while for the node problem this is denoted at $v_{c,b}^{(d)}$, where the superscript indicates the dimensionality of the grid.

The critical behavior of the quantities characterizing the percolation grid is described in the following form [1]:

the relative number of nodes belonging to the IC:

$$P(v) \sim (v - v_c)^{\beta}, \quad v > v_c, \tag{1}$$

the average number of nodes in the finite cluster

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$$S \sim (v - v_c)^{-\gamma}, \tag{2}$$

the correlation length ξ which characterizes the dimension of the finite cluster when $v < v_c$ and the dimensions of the voids in the IC when $v > v_c$:

$$\xi \sim |v - v|^{-\nu}. \tag{3}$$

The critical indices β, t, γ, ν are universal (they depend only on the dimensionality d of the grid) and satisfy the relationship

$$\nu = (2\beta + \gamma)/d. \tag{4}$$

The percolation theory was recently enhanced through the concept of fractal dimensionality, which is related to geometric objects exhibiting fractional dimensionality [4, 5]. The concept of the fractal arose in mathematics, in particular in the construction of continuous functions, that had no derivatives at any point (for example, the path of a Brownian particle), and in the conception of curves which entirely fill a square [4].

If the length L is defined in the form of [5]:

$$L = a\left(\frac{R}{a}\right)^D,$$

then the parameter D is referred to as the fractal dimensionality:

$$D = \frac{\lg L/a}{\lg R/a}. \tag{5}$$

where a is the magnitude of the scale being utilized here; R is the distance between the points on the straight line connecting the ends of the fractal object.

PERCOLATION GRID MODEL

In the first stage of the calculations we determined the conductivities of the linkage in the generalized nodes on the basis of an elementary cell in the form of $n \times n$ for the plane case and in the form of $n \times n \times n$ for the three-dimensional case. In the second stage the grid is constructed with chaotic distribution of the generalized nodes (obtained in the first calculation stage) for the rectangular grid of the elementary cell, where identical dimensionality for the generalized nodes and the grid is maintained, i.e., the linkages in the elementary cell are replaced by finite grids whose parameters are determined in the preceding calculation stage. This procedure for grid growth is repeated in the subsequent stage. The number of stages is limited by the condition of independence for the effective grid properties relative to the calculation stage.

Let us examine in greater detail the algorithm for determining the parameters of the percolation grid in the second stage which is universal for the following (i + 1) stages. We will then describe the difference between the first stage from the remaining stages.

First Step. We introduce the conductivity combination (of generalized nodes) and their random scattering over the linkages; a special combination of nodes is formed.

Second Step. We then encompass the nodes of the side surface (edge) from which the calculation proceeds; we isolate the linkages and recall the nodes connected to the generalized node in the special combination.

Third Step. We encompass the nodes which have been isolated in the special combination during the first step, we fix the linkages of these nodes and recall the new nodes connected to the generalized nodes. The third step is repeated until the memory combination is entirely filled with zeros, i.e., until all of the linkages of the cluster have been taken into consideration, and we have reference to those which reach the side surface (this combination was formed in the first step).

Fourth Step. We now undertake a test of whether or not we have penetration to the opposite surface (exit)? If there is no penetration, this becomes fixed and new scattering is undertaken, with transition to the start of the program. If there is penetration, we execute transition to the following step.

Fifth Step. We compile the equations for flow conservation (equilibrium) for the nodes of the IC frame.

DETERMINATION OF CONDUCTIVITY

For the conductivity problem, according to the Kirchhoff law, for the inside nodes (not belonging to the two boundary surfaces) we obtain

$$\Big(\sum_{i=1}^{k}\sigma_{ji}\Big)U_j-\sum_{i=1}^{k}\sigma'_{ji}U_i=0, \tag{6}$$

for the nodes belonging to the first boundary surface F_1, the conservation equation has the form

$$\Big[\Big(\sum_{i=1}^{k}\sigma_{j_1\,i}\Big)+S\Big]U_{j_1}-\sum_{i=1}^{k}\sigma_{j_1\,i}U_1=SU_0^{(1)}, \tag{7}$$

for the nodes belonging to the second boundary surface F_2:

$$\Big[\Big(\sum_{i=1}^{k}\sigma_{j_2\,i}\Big)+S\Big]U_{j_2}-\sum_{i=1}^{k}\sigma_{j_2\,i}U_i=SU_0^{(2)}. \tag{8}$$

We have introduced the following notation here: S, the average conductivity of the previous stage; σ_{ij}, the conductivity of the linkages between the i-th and j-th nodes; k, the number of linkages for the j-th node; U_i, the potential of the i-th node; $U_0^{(1)}$, the average potential of the surface F_1; $U_0^{(2)}$, the average potential of the surface F_2; j_1, j_2, the numbers of the nodes belonging to surfaces F_1 and F_2, respectively.

The effective conductivity for the given scattering of linkages in the percolation grid is found from the formula

$$\sigma_n=\sum_{i=1}^{l}\frac{(U_i-lU_0^{(1)})(m+1)}{(U_0^{(2)}-U_0^{(1)})m}S, \tag{9}$$

where ℓ represents the number of nodes on the surface F_1; m is the number of nodes at the edge of the cell.

Sixth Step. Return to the start of the program and repetition of the first five steps with a new scattering of linkages through the grid. The entire scattering number for the given concentration of linkages will subsequently be assumed to be equal to N = 16.

The average conductivity σ for the percolation grid in the case of N scatterings is determined from the formula

$$\sigma=\frac{1}{N}\sum_{n=1}^{N}\frac{\Big(\sum_{i=1}^{d}\sigma_n^{(i)}\Big)}{d}, \tag{10}$$

where n represents the scattering number.

The critical behavior of σ is described in accordance with the following formula:

$$\sigma\sim(v-v_c)^t\ . \tag{11}$$

The difference in the first stage (i = 1) from i + 1 involves the following: 1) the linkages are disrupted in random fashion (removal of the nodes), and the conductivity of the hole linkages is equal to 1; 2) in the Kirchhoff equations (7) and (8) the quantity S = 1.

DETERMINATION OF THE PENETRATION THRESHOLD

Let us introduce the following notation: $P_{c,s}^{(d)}$ is the fraction of nondisrupted linkages; $P_b^{(d)}$ is the fraction of nodes belonging to the IC.

The penetration threshold $v_{c,s}^{(d)}$ is determined from the condition

TABLE 1. Results from Research on a Two-Dimensional Grid

Linkage problem				Node problem			
v	D	$P(x)$	σ	v	D	$P(x)$	σ
0,99	2	1	1	0,99	1,953	0,99	0,981
0,89	2	1	0,866	0,89	1,914	0,89	0,738
0,79	1,996	0,995	0,7	0,79	1,817	0,79	0,526
0,69	1,93	0,86	0,5	0,69	1,649	0,69	0,231
0,59	1,751	0,803	0,13	0,68	1,634	0,68	0,202
0,58	1,732	0,78	0,1	0,67	1,598	0,661	0,079
0,57	1,683	0,752	0,081	0,66	1,562	0,613	0,0117
0,56	1,707	0,725	0,069	0,65	1,546	0,606	0,0111
0,55	1,686	0,695	0,05	0,64	1,535	0,57	0,00186
0,54	1,697	0,653	0,03	0,63	1,515	0,55	0,0015
0,53	1,696	0,583	0,0125	0,62	1,477	0,532	0,0011
				0,61	1,452	0,489	0,0007
				0,6	1,44	0,418	0,00025

TABLE 2. Results from Research on a Three-Dimensional Grid

Linkage problem				Node problem			
v	D	$P(v)$	σ	v	D	$P(v)$	σ
0,99	3	1	0,99	0,99	2,993	0,99	0,982
0,89	3	1	0,882	0,89	2,916	0,89	0,779
0,79	2,998	1	0,774	0,79	2,828	0,79	0,583
0,69	2,999	1	0,579	0,69	2,721	0,69	0,407
0,59	2,763	0,734	0,0983	0,59	2,591	0,59	0,26
0,49	2,617	0,6312	0,0873	0,49	2,363	0,48	0,127
0,39	2,55	0,446	0,068	0,39	1,961	0,372	0,035
0,36	2,391	0,433	0,0213	0,38	1,931	0,363	0,024
0,35	2,44	0,442	0,0063	0,37	1,874	0,254	0,00656
0,34	2,418	0,436	0,0054	0,36	1,852	0,228	0,00323
0,33	3,393	0,414	0,00145	0,35	1,824	0,194	0,00111
0,32	2,383	0,406	0,0013	0,39	1,8	0,15	0,00115
0,31	2,323	0,383	0,00114	0,33	1,677	0,137	$1{,}255\cdot 10^{-5}$
0,30	2,179	0,35	0,00119	0,32	1,644	0,118	$7{,}38\cdot 10^{-6}$
0,29	2,196	0,33	0,0011	0,31	1,56	0,087	$2{,}19\cdot 10^{-6}$
0,28	2,119	0,31	0,00109	0,30	1,546	0,072	$2{,}727\cdot 10^{-9}$
0,27	2,071	0,28	0,00062				
0,26	2,003	0,235	0,00033				
0,25	2,013	0,177	0,00009				

TABLE 3. Critical Indices of Percolation Grid

Index	$d=2$	$d=3$
β	0,14±0,03 0,138±0,007 0,148±0,004 0,14±0,01*	0,35±0,05 0,39±0,02 0,47±0,02 0,40±0,01*
t	1,10±0,10 1,15±0,15 1,10±0,10 1,12±0,02*	1,725±0,005 1,60±0,1 1,75±0,1 1,7±0,02*

Note. The asterisk identifies the authors' data.

TABLE 4. Penetration Thresholds for Rectangular Percolation Grid

Penetration threshhold	$d=2$	$d=3$
$v_{c,b}$	0,50 0,493±0,013 0,498±0,017 0,520±0,02*	0,247±0,05 0,240±0,01*
$v_{c,s}$	0,590±0,01 0,581±0,001 0,591±0,001 0,595±0,02*	0,304±0,01 0,320±0,001 0,299±0,001*

Note. The asterisk identifies the authors' data.

TABLE 5. Fractal Dimensionality of IC Near Penetration Threshold

Model	$d=2$	$d=3$
Cluster-cluster	1,44±0,04	1,77±0,03
Particle-cluster	1,68±0,02	2,46±0,05
Percolation grid linkage problem	1,69±0,002	2,013±0,002
Node problem	1,515±0,002	1,546±0,002

$$\lim_{n\to\infty} P_n^{(d)} = \begin{cases} 1, & \text{if} \quad P_{1,s}^{(d)} > v_{c,s}^{(d)}, \\ 0, & \text{if} \quad P_{1,s}^{(d)} < v_{c,s}^{(d)}, \end{cases} \tag{12}$$

where n is the number of stages.

In this case, for the linkage problem we have satisfied:

$$\begin{aligned} &\text{if} \quad P_N(i) > P_s^{(d)}, \quad P_s^{(d)} > v_{c,s}^{(d)}, \\ &\text{if} \quad P_N(i) \leqslant P_s^{(d)}, \quad P_s^{(d)} \leqslant v_{c,s}^{(d)}, \end{aligned} \tag{13}$$

where $P_N(i)$ is the relative IC number over all possible realizations in the i-th stage.

Thus, reducing $P_s^{(d)}$ from 1 to 0, we find $v_{c,s}^{(d)}$ as the value of the volumetric concentration of linkages at which (13) becomes valid.

For the node problem we satisfy:

$$\begin{aligned} &\text{if} \quad P_N(i) > v_{c,s}^{(d)}, \quad P_b^{(d)} > v_{c,b}^{(d)}, \\ &\text{if} \quad P_N(i) < v_{c,s}^{(d)}, \quad P_b^{(d)} < v_{c,b}^{(d)}. \end{aligned} \tag{14}$$

This is a consequence of the fact that the node problem in the second stage changes into a linkage problem. Having reduced $P_b^{(d)}$ from 1 to 0 and knowing $v_{c,s}^{(d)}$, we can determine $v_{c,b}^{(d)}$ in accordance with (14).

DETERMINATION OF THE FRACTAL DIMENSIONALITY

The number of nodes in the IC, referred to the entire number of nodes in the grid, was determined in accordance with the formula

$$P(x) = \prod_{P_N(i-1)} P_s(i), \tag{15}$$

where $P_s(i)$ is that fraction of nodes belonging to the IC found in the i-th stage of the calculations.

The quantity $P_N(i-1)$ in the first stage ($i = 1$) assumes the following values: $P_N(0) = P_b^{(d)}$ for the node problem; $P_N(0) = P^{(s,d)}$ for the linkage problem. $P_s(i)$ and $P_N(i)$ in the i-th stage of the calculation are defined as the concentrations of the hole linkages, equal to $P_N(i-1)$, i.e., to the relative number of IC.

In each calculation stage entire cells of the previous stage drop out of the IC grid $[(m-1)^i + 1]^d$, since a portion of these are no longer connected to the IC.

The fractal dimensionality of the cluster was calculated in accordance with the formula

$$D = \frac{\sum_{(V)} (\ln P_s(i)/\ln m)}{L}, \tag{16}$$

where L is the number of the IC in all scatterings with the numbers j. Summation in the parentheses is carried out over the set V, where V is the set of all IC for N scatterings (the power is equal to L).

The calculation results with the described scheme are found in Tables 1 and 2. Tables 3 and 4 show comparison of the calculation results for β, t, $v_{c,b}^{(d)}$ and $v_{c,s}^{(d)}$ in the case of the percolation grid being studied here, as well as the data derived by other authors [1]. The calculated penetration threshold $v_{c,s}^{(d)}$, $v_{c,b}^{(d)}$, the critical indices t, ν are in good agreement with the data in the literature [1-5]. This may serve as confirmation of the usefulness of the proposed mathematical model of the percolation grid in which it is possible to study both structural and physical properties of percolation systems.

Table 5 shows a comparison of the calculated fractal dimensionality of the IC, derived in a percolation grid near the penetration threshold, following the "cluster-cluster" and "particle-cluster" schemes [3-5]. It follows out of this comparison (Table 5) that with the aid of all three models IC are formed with various fractal dimensionalities.

CONCLUSION

We have developed a mathematical model of two- and three-dimensional percolation grids. The calculated critical indices β, t and the penetration thresholds for the node and linkage problems are in good agreement with the literature data.

We have determined the fractal dimensionality D of an infinite cluster obtained on a two- and three-dimensional percolation grid for the node and linkage problems.

NOTATION

v, volumetric concentration of hole linkages; $v_{c,s}$, penetration threshold for linkage problem; $v_{c,b}$, penetration threshold for node problem; β, critical index for IC density; γ, critical index for finite cluster; ν, critical index for correlation length; d, grid dimensionality; D, fractal dimensionality; σ, conductivity; U, potential; t, critical index for conductivity; P, fraction of nodes belonging to the IC.

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