Percolation threshold of a simple cubic lattice with fourth neighbors: the theory and numerical calculation with parallelization

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Abstract. The method of finding a percolation threshold x_c of infinite lattice in the problem of nodes is proposed. Theoretically was shown that curves of conditional probability of percolation of finite lattices are intersected in the critical point x_c. The method has been implemented in numerical experiment with parallelization on a finite simple cubic lattice for coordination numbers $Z = 6; 8$ and 12. Experimental curves of conditional probability of percolation Y were built (x, L) for lattice sizes $L = 32; 64; 128$ and 256 for case of interaction with second $(Z = 12)$ and third $(Z = 8)$ neighbors. For interaction with fourth $(Z = 6)$ neighbors $L = 33; 65; 127$ and 255 as obvious feature was found — zero probability of lattice percolation if lattice size is even number. The assessment of percolation threshold of a simple cubic lattice with the fourth neighbors $x_c = 0.3115$, being conformed with known value of percolation threshold with the first neighbors was received.

Keywords

Keywords: lattice, site problem, simple cubic, percolation threshold, parallelization.

1 Introduction

Numerical modeling of physical processes in view of limited opportunities of any computer are carried out on lattices of final sizes. In the lattice percolation theory the two-phase system is allocated randomly on N nodes (connections) of regular lattice of dimensionality d, and concentration or part of nodes (connections) of conducting phase is equal to x. x_c concentration below which percolation is absent, is named a critical concentration or a percolation threshold. The knowledge of x_c is an important applied value of the percolation theory at modeling a wide class of phenomena: magnetic phase transitions, charge and substance transfer, formation of gels, distribution of epidemics, fires, etc. It isn't possible to specify all applications of the percolation theory here as this list grows over time. For example, percolation appeared convenient model, as for description of galactic structures, and network safety on the Internet.

More than half a century passed from Florey's works [1] and Stockmayer [2], and later on Broadbent and Hammersly [3], however methods of analytical solution of percolation problems (including methods of x_c calculation) are still unknown. Percolation thresholds at $d = 2$ are precisely known only for several lattices [4]. The majority of works on definition of x_c of lattices at $d \geq 2$ are based on numerical methods or approximate theoretical models [5 - 16].

At $2d$ and $3d$ computer simulation the practical interest present square and simple cubic lattices. For square lattice at interaction with first $(N2)$ neighbors (coordination number $Z = 4$) $x_c = 0.592746\ldots$ was obtained in [7], and for simple cubic lattice $x_c = 0.311608\ldots$ was received in [10] also at interaction with first $(N2)$ neighbors $(Z = 6)$.

The numerical investigation of percolation threshold in the problem of percolation of knots (sate problem) of square lattice at altering number of neighbors Z was conducted in [13]. The identical percolation thresholds $x_c = 0.592\ldots$ was found by the Monte-Carlo method for $Z = 4$ found identical thresholds at interaction with the

first ($N2$), second ($N3$), third ($N4$) and fifth ($N6$) neighbors. Then various combinations of ranges considered interaction ($N2 + N3$), ($N2 + N4$), ($N2 + N3 + N4$) and ($N2 + N5$). Calculated the percolation threshold, respectively, are as $x_c = 0.407\ldots, 0.337\ldots, 0.288\ldots, 0.234\ldots$ for $Z = 8$. Therefore authors draw a conclusion that coordination number and dimension of space are not enough to predict the percolation threshold of a lattice by the "a universal formula", offered in [17]. However the result in [13] prompts that identical percolation thresholds are apparently possible at identical Z. Whether the same is possible in space of bigger dimension, for example at $d = 3$?

At $d = 3$ numerical research of percolation thresholds is conducted in [15] for a simple cubic lattice at interaction with the second ($Z = 12$, further $sc2$) and the third ($Z = 8$, further $sc3$) neighbors. Identical percolation thresholds as in the case with square lattice were not revealed. Apparently, as in case with square lattice, at $d = 3$ identical thresholds may be expected at identical Z. It is easy to see that a simple cubic lattice with the first neighbors ($sc1$) and the fourth neighbors are characterized by identical $Z = 6$. For a lattice $sc1$ the result $x_c = 0.3116\ldots$ except [10] is confirmed even in several researches. However for a simple cubic lattice with the fourth neighbors ($sc4$) us not aware of any work. Therefore research of percolation properties and an assessment percolation threshold value of this lattice are the main objective of the present work.

2 Method theory

The percolation probability or probability that randomly chosen knot of lattice of size L belongs to a connecting cluster $P(x, L)$ is connected with function of conditional probability of percolation of lattice $Y(x, L)$ as $P(x, L) = xY(x, L)$.

reliminary theoretical studying and extensive modeling [18] show that function of conditional probability of percolation of lattice $Y(x, L)$ may be presented as

$$Y(x, L) = \frac{1}{1 + e^{-S(x,L)}}, \quad \text{where} \quad S(x, L) = \sum a_i(x_i - x_{cL}^i), \tag{1}$$

where x_{cL} correspond to condition $Y(x_{cL}, L) = 0.5$, a_i — coefficients of power series depending on i index, which changes at summation from 1 till $n = N_{max} - N_{min}$, N_{min} — a minimal number of knots-conductors, at which appearance of connecting cluster N_{max}, corresponding to the maximal number of nodes-conductors at which connecting cluster may absent.

Consider $S(x, L) = \sum a_i(x_i - x_{cL}^i)$ close to x_{cL}. At $x \approx x_{cL}$ or small $|x - x_{cL}|$ the $\sum S(x, L)$ may be presented with one summand :

$$S(x, L) = \sum a_i(x_i - x_{cL}^i) = (x - x_{cL})(a_1 + a_2 2x_{cL} + \ldots + a_n n x_{cL}^{n-1}) = A_L(x - x_{cL}). \tag{2}$$

Then in order to set $Y(x, L)$ function at small $|x - x_{cL}|$ two parameters A_L and x_{cL} are sufficient:

$$Y(x, L) = \frac{1}{1 + e^{-A_L(x - x_{cL})}} \tag{3}$$

at this A_L corresponds to slope K :

$$K = A_L/4 \tag{4}$$

of tangential $y(x)$:

$$y(x) = \frac{1}{2} + K(x - x_{cL}), \tag{5}$$

to curve $Y(x, L)$ in the point x_{cL}, as

$$K(x) = (a_1 + 2a_2 x + \ldots + n a_n x^{n-1}) Y(x)(1 - Y(x)) \tag{6}$$

In the general case close to the critical point $x \approx x_c$ for lattice with linear size L the skyling relationship is valid via the critical index of correlation radius ν, which in the three-dimensional case is in the order of unit $\nu \approx 1$ [9]:

$$|x - x_c|^{-\nu} \propto L \quad \text{or} \quad |x_{cL} - x_c|^{-\nu} \propto L, \tag{7}$$

So at $\nu \approx 1$ one can write for three-dimensional lattices:

$$x_{cL} = x_c + \frac{B}{L}, \tag{8}$$

where B — is a constant. It follows from (7) and (8) that

$$x_c - x_{cL} = B_1/L \quad \text{or} \quad x_c - x_{cL} = B_\nu/L^{1/\nu} \tag{9}$$

where B_1 and B_ν — are coefficients of proportionality.

Then at $x_c = const$ increase of the lattice size L brings to alteration of x_{cL}, in such way that at $L \to \infty$, $x_{cL} \to x_c$.

If to take $x = x^*$ in (5), then subtracting $y(x^*) = 1/2 + K(x^* - x_{cL})$ from (5), we receive an equation of sheaf of lines, propagating through the sheaf center with coordinates x^* and $y(x^*)$:

$$y(x) - y(x^*) = K(x - x^*), \tag{10}$$

notably all tangentials (5) to curves $Y(x, L)$, transmitted through the point with coordinates x_{cL} and $Y(x_{cL}, L) = 1/2$, are intersected in one point at $x = x^*$. Ratio of first and second from (7) at $x = x^*$ brings

$$|(x^* - x_c)/(x_{cL} - x_c)| = 1,$$

whence $x^* = x_{cL}$ may be at $L \to \infty$, notably when $x^* \to x_c$. Thus, take the intersection point of tangential (5) to curves Y(x,L) as a critical point $x^* = x_c$. Whence follows, that for lattice under consideration $K(x_c - x_{cL}) = y(x_c) - 1/2$ or

$$K(x_c - x_{cL}) = (A_L/4)(x_c - x_{cL}) = const, \tag{11}$$

then and $Y(x, L)$ functions will intersect in the critical point with coordinates $x = x_c$ and $Y_c = Y(x_c) = const$, though $Y(x_c)$ is determined as $Y(x_c, L) = \frac{1}{1+e^{-A_L(x-x_{cL})}}$ and according to (11) receive

$$Y(x_c, L) = \frac{1}{1 + e^{-A_L B_1/L}} = const \quad \text{or} \quad Y(x_c, L) = 1/(1 + exp^{-A_L B_\nu/L^{1/\nu}}) = const \tag{12}$$

For fulfillment of (12) A_L variable is to grow at increase of the lattice size L as $A_L \propto L^{1/\nu}$, at that for three-dimensional lattices according to the first from of (9) as

$$A_L \propto L. \tag{13}$$

3 Computer experiment and its features

Lets receive expressions, by which the lattice functions $A_L = A_L(L)$ and $x_{cL} = x_{cL}(L)$ may be determined from the computer experiment. For this use results of integration of functions $Y(x, L)$ and $X(x, L)$ in the limits interesting to us [18]:

$$I_1 = \int_0^1 Y(x, L)dx = 1 - x_{cL} \tag{14}$$

as well as

$$I_2 = \int_0^{x_{cL}} Y(x, L)dx = \ln 2/a_1(L) \tag{15}$$

$$I_3 = \int_{x_{cL}}^1 Y(x, L)dx = 1 - x_{cL} - \ln 2/a_1(L) \tag{16}$$

$$S_3 = \int_0^{x_{cL}} (1 - Y(x, L))dx = \ln 2/a_1(L) \tag{17}$$

it was taken at integration that for $L > 2$

$$e^{-A_L(L)(1-x_{cL})} \ll 1 \quad \text{and} \quad e^{A_L(L)x_{cL}} \gg 1, \tag{18}$$

The integrals $I1$, $I2$ and $I3$ express areas under the curve $Y(x, L)$ at corresponding limits, and integral $S3$ — area under the curve $Y(x)$. Therefore replacing integral $I1$ over (14) by the finite sum, one can determine x_{cL} to a nicety for lattice of L size by the experimental points x_i, $Y_i(x_i)$

$$x_{cL} = 1 - (1/2)\sum_{i=1}^{k}(x_{i+1} - x_i)(Y_{i+1} - Y_i) \tag{19}$$

where k may take maximal value $k_{max} = 1/h_{min}$, if $h_{min} = 1/L^3$ — is a minimally possible step by x.

Each experimental value $Y_i(x_i)$ was determined from computer tests by the Monte-Carlo method:

$$Y_i(x_i) = N_x/N, \tag{20}$$

where N — total value of two-phase systems (generated in the process of computer experiment) in statistical ensemble, N_x — number of systems in ensemble in which the connecting cluster was formed at the given value of x and size L of simple cubic lattice.

Notice, that each two-phase system of statistical ensemble consists of conducting and nonconducting phases randomly distributed on L^3 nodes of simple cubic lattice, and x — it is part of nodes of phase interesting to us.

For experimental defining of AL lets replace sum of integrals I2 and S3 by the finite sum I2 + S3 =S in form

$$S = \frac{1}{2}\sum_{i=1}^{m}(x_i + 1{-}x_i)(Y_{i+1} + Y_i) + \sum_{j=1}^{m}(x_{j+1}{-}x_j)(X_{j+1} + X_j), \tag{21}$$

where $m = x_{cL}/h_m, n = (1 - x_{cL})/h_n, h_m$ — is step along x in the range from 0 till x_{cL}, and X_{j+1} and X_j are determined from connection $X(x, L) = 1 - Y(x, L)$ in the range from x_{cL} till 1 with step h_n. The region of appreciable changing of function $Y(x, L)$ we will characterize by the width of transition $\Delta x = 4/A_L$, then in order to reach maximum precision of computer experiments it is necessary that steps h_m and h_n were minimal in the region $\Delta x : h_{min} = 1/L^3$.

Having determined the amount of S by (21) we find the experimental value of the A_L :

$$A_L = 2\ln 2/S, \tag{22}$$

Knowledges of x_{cL} and A_L allow to build the smoothing function by the formula (3)

$$Y(x, L) = \frac{1}{1 + e^{-A_L(x - x_{cL})}}$$

In computer experiments the number of systems in statistical ensemble was set in the range of 10^4 to 10^6 in dependence on the lattice size L.

Let's turn to features of the computer experiment. For calculation of percolation threshold and the medium size of of finite cluster of cubic lattices the cluster marking of Hoshen-Kopelman [19], described in the literature for the square lattice. The given algorithm is considered as one of the best as it allows to calculate several characteristics at once. In our work the variant of algorithm is used where the random lattice is generated as a whole, what allow to find more exact values of percolation characteristics.

Simulation of cubic lattices with different connections (such as with fourth neighbors, $Z = 6$) requires modification of one from blocks of classic algorithms, with the aim of taking these connections into account. If occupied cell of cluster (notice its belonging to cluster k), connects more than two marked clusters: $k_1, k_2, \ldots, k_n$, then function of re-marking $m(k_1, k_2)$ is performed sequentially $n - 1$ times. This means that $k = m(k1, m(k2, \ldots m(k_{n-1}, k_n))$, where function $m(k_1, k_2)$ marks all cells of cluster k_2 with number of cluster k_1 and returns number of the last.

For the lattice with four neighbors ($Z = 6$) it is also necessary to take into account the distance between cells possessing connection, in the given case it is equal to 2. Therefore at marking it is necessary to consider a "neighbor" if the current cell is situated on the distance not less than two from the lattice edge correspondingly on the left, on the top and on behind. One more obvious feature of a lattice with the fourth neighbors is the zero percolation probability if size of a lattice is even number for any distributions of occupied cells. Therefore minimal nontrivial lattice size $L = 3$ with number of nodes $N = L^3 = 27$.

Important point in computing experiment by a method of statistical tests is the right choice of a random number generator. In practice generators of real random numbers have very low productivity therefore their use in this task and in mathematical modeling in general, is limited. It is possible to choose boost/random library in which there are some algorithms with different characteristics from existing realization of generators of pseudorandom numbers. In our case the most important are the cycle length, good multidimensional distribution, and also satisfactory productivity. For generation of casual distribution of cells in a lattice mt19937 is chosen from offered generators, with a cycle $2^19937 - 1$ and good uniformity to 623 measurements. This allows to receive several parallel consequences of random numbers, for this aim it is necessary to set different initial parameters, for example $t, t + 1, \ldots, t + p - 1$, where t — time of returned system function time(), p —number of calculators.

Computing experiment for qualitative assessments requires a big calculation time therefore usually at solution of such tasks the methods of parallel or distributed programming are used. For today one of the widely used mechanisms is the interface of data exchange (MPI standard). Sizes of the calculated lattices allocated completely in memory, are limited to the size of operational memory itself, that as a rule, allows to calculate the cubic lattices with side L no more than 500. At such sizes calculation of one lattice of one size L on one kernel of the modern processor as a rule doesn't exceed several minutes or even seconds. Therefore distributions of calculations within one model it isn't required. Therefore, parallelization of calculations consists in distribution of the set number of models of lattices on processors. Models casual also are generated directly on the processor which is carrying out calculation of characteristics. Data exchange at such distribution is insignificant and doesn't influence productivity. Then any realization of MPI and the usual local Ethernet network can be used.

In this work the calculations were used, which have been executed on the couple on separate computers in the local net: processor Q6600 4 cores, 4GB, and also cluster of two-processors blade servers, 7 nodes in total. Operational system Debian GNU/Linux 6.0, gcc compiler, the Boost library.

4 Discussion of results

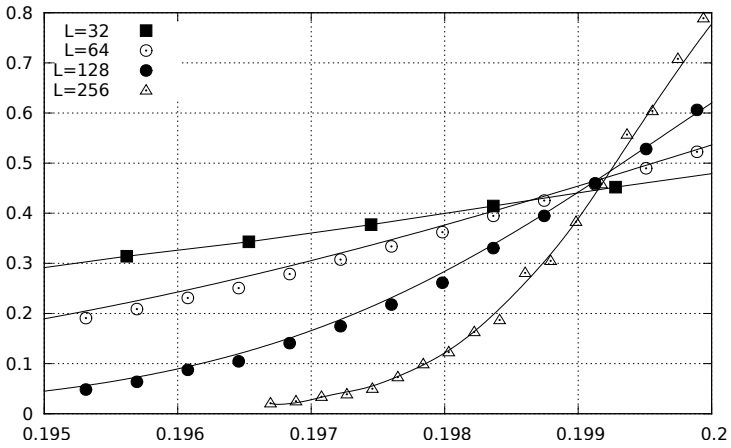

Figure 1. Experimental points $Y_i(x_i, L)$ simple cubic lattice sc3 ($Z = 8$) for sizes $L = 32, 64, 128$ and 256 are smoothed out by the solid curves $Y(x, L)$ by (3). The percolation threshold is within the range of the points of intersection, from 0.1988 to 0.1992, which is consistent with $x_c = 0.1991(1)$ [15].

The main results of work are presented graphically on the fig.1–fig.3. It is shown on the pictures, that smoothing (solid curves) and experimental functions $Y_i(x_i, L)$ are practically coincide. As a measure of non-coincidence (error) of experimental dependence $Y_i(x_i, L)$ from suggested $Y(x, L)$ by (3) the standard deviation $c_{YL} = \sqrt{D_{YL}}$ is used, where $D_{YL} = \overline{(\Delta Y_L)^2}$ — is dispersion calculated for non-trivial points of random (experimental) function $Y_i(x_i, L)$. So for our lattice (sc4) $L = 33; 65; 127$ and 255 the corresponding values of standard deviations were received $c_{Y33} = 0.024$; $c_{Y65} = 0.017$; $c_{Y127} = 0.011$; $c_{Y255} = 0.004$. On the base of even such " pessimistic" (overrated) assessment of standard deviations one can say that theory and experiment are agree with each other. To estimate the percolation threshold we chose the intersection of smoothed through (3) of the curves with the lowest values c_{YL}. In our case (fig.3.) to the point of intersection x_c of curves $Y(x, L)$ for simple cubic cell with forth neighbors at $L = 127$ and $L = 255$ the value 0.3115 corresponds, nicely agree with percolation threshold for simple cubic lattice with first neighbors (sc1) $x_c = 0.3116\ldots$ [10]. At this the compared lattices have identical coordination numbers $Z = 6$.

5 Conclusions

1. The model of behavior of conditional probabilities of percolation $Y(x, L)$ allows to introduce the concept of critical point x_c (percolation threshold) for infinite lattice as point of intersection of curves by (3).

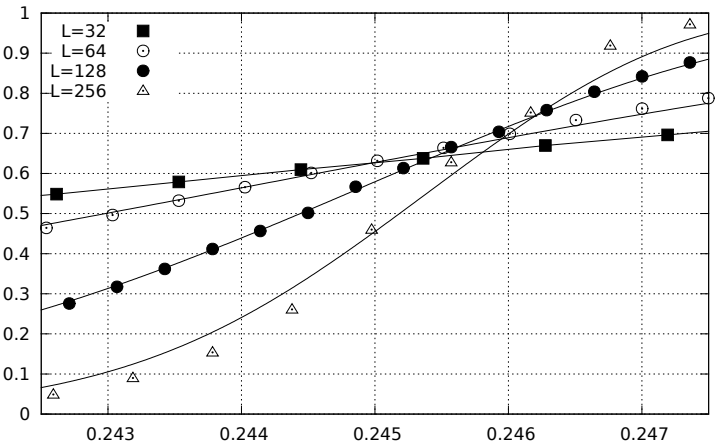

Figure 2. Experimental points $Y_i(x_i, L)$ simple cubic lattice sc3 ($Z = 8$) for sizes $L = 32, 64, 128$ and 256 are smoothed out by the solid curves $Y(x, L)$ by (3). The percolation threshold is within the range of the points of intersection, from 0.2450 to 0.2463, which is consistent with $x_c = 0,2455(1)$ [15].

2. To receive curves $Y(x, L)$ the problem of experimental definition by the Monte-Carlo method the values of function of conditional percolation probability at parallelization of calculations of set number of lattice models by processors was solved.

3. For assessment of percolation threshold it is ought to take the point of intersection of two smoothed curves $Y(x, L)$ with lowest values of standard deviation c_{YL}.

4. The experimental assessment of value of percolation threshold received in this work $x_c = 0.3115$ for simply cubic lattice with fourth neighbors ($Z = 6$) is nicely agree with value of percolation threshold for simple cubic lattice with first (also $Z = 6$) neighbors.

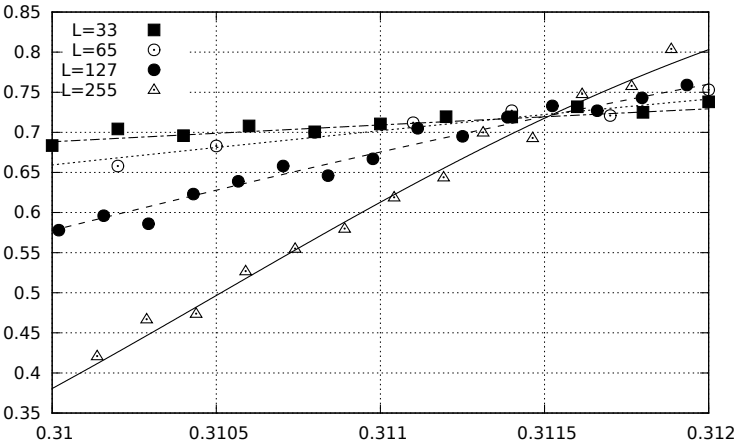

Figure 3. Experimental points $Y_i(x_i, L)$ simple cubic lattice sc4 ($Z = 6$) for sizes $L = 33, 65, 127$ and 255 are smoothed out by the solid curves $Y(x, L)$ by (3). The point of intersection, smoothed by (3) of the curves with the lowest values Y_L for $L = 127$ and $L = 255$, corresponds to the value of 0.3115, which is consistent with $x_c = 0,311608\ldots$ [10] for a simple cubic lattice sc1 ($Z = 6$).

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