Simple cubic random-site percolation thresholds for neighborhoods containing fourth-nearest neighbors

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In the paper random-site percolation thresholds for simple cubic lattice with sites’ neighborhoods containing next-next-next-nearest neighbors (4NN) are evaluated with Monte Carlo simulations. A recently proposed algorithm with low sampling for percolation thresholds estimation [Bastas et al., arXiv:1411.5834] is implemented for the studies of the top-bottom wrapping probability. The obtained percolation thresholds are \( p_c(4\text{NN}) = 0.31160(12) \), \( p_c(4\text{NN}+2\text{NN}) = 0.15040(12) \), \( p_c(4\text{NN}+2\text{NN}+\text{NN}) = 0.115950(12) \), \( p_c(4\text{NN}+3\text{NN}) = 0.20490(12) \), \( p_c(4\text{NN}+3\text{NN}+\text{NN}) = 0.11920(12) \), \( p_c(4\text{NN}+3\text{NN}+2\text{NN}) = 0.11330(12) \), \( p_c(4\text{NN}+3\text{NN}+2\text{NN}+\text{NN}) = 0.10000(12) \), where 3NN, 2NN, NN stands for next-next-nearest neighbors, next-nearest neighbors, and nearest neighbors, respectively. As an SC lattice with 4NN neighbors may be mapped onto two independent interpenetrated SC lattices but with two times larger lattice constant the percolation threshold \( p_c(4\text{NN}) \) is exactly equal to \( p_c(\text{NN}) \). The simplified Bastas et al. method allows for reaching uncertainty of the percolation threshold value \( p_c \) similar to those obtained with classical method but ten times faster.

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INTRODUCTION

Finding percolation thresholds \( p_c \) and observing cluster properties near percolation threshold [1–4] are one of the most extensively studied problems in statistical physics. The beauty of percolation [5] lays both in its simplicity and possible practical applications. The latter ranges from theoretical studies of geometrical model of the phase transition [6], via condensed matter physics [7], rheology [8], forest fires [9] to immunology [10] and quantum mechanics [11].

In random-site percolation model the nodes of lattice, graph or network are randomly occupied with a probability \( p \). The critical probability \( p_c \) separates two phases: for \( p > p_c \) the system percolates, i.e. one may find a single cluster of occupied sites which extends to the borders of the system; while for \( p < p_c \) only smaller clusters exist. Usually, the finite size scaling theory [12–15] is employed for percolation threshold \( p_c \) estimation. This requires checking properties of some quantity \( X(p, L) \) in the vicinity of phase transition as it depends on the linear system size \( L \)

\[
X(p; L) = L^{-\frac{\nu}{\beta}} \cdot F((p - p_c) L^{1/\nu}),
\]

where \( F(\cdot) \) is a scaling function, \( x \) is a scaling exponent and \( \nu \) is a critical exponent associated with the correlation length [1]. Eq. (1) yields an efficient way for \( p_c \) determination as \( L^x \cdot X(p_c; L) = F(0) \) does not depend on the linear system size \( L \). It means that curves \( L^x \cdot X(p; L) \) plotted for various values of \( L \) should have one common point exactly at \( p = p_c \). Unfortunately, the results of computer simulations rather rarely reproduce a single common point of curves \( X(p; L) \) unless the number \( N_{\text{run}} \) of prepared lattices is very high.

Recently, Bastas et al. proposed efficient method for estimating scaling exponents \( x \) and percolation thresholds \( p_c \) in percolation processes with low sampling [16, 17]. According to Refs. [16, 17] instead of searching for the point when curves \( X(p; L) \) intercept each other one may wish to minimize the pairwise difference

\[
\Lambda(p; x) = \sum_{i \neq j} [H(p; L_i) - H(p; L_j)]^2,
\]

with respect to both parameters \( x \) and \( p \), where

\[
H(p; L) \equiv Y(p; L)
\]

(3a)

as suggested in Ref. [16] or

\[
H(p; L) \equiv Y(p; L) + 1/Y(p; L)
\]

(3b)

as proposed in Ref. [17] and in both cases

\[
Y(p; L) \equiv L^x \cdot X(p; L).
\]

The minimum of \( \Lambda(p; x) \) is reached for \( p = p_c \) and \( x = \beta/\nu \), where \( \beta \) is a critical exponent associated with the order parameter (for instance probability of an arbitrary site belonging to the infinite cluster [1]).

In this paper we propose simplified version of Bastas et al. algorithm, where only a single-parameter function \( \lambda(p) \) must be minimized in order to provide percolation threshold estimation. With such approach we estimate simple cubic (SC) random-site percolation thresholds for
eight complex neighborhoods containing next-next-next-nearest neighbors. Our results enhance those of the earlier studies regarding percolation thresholds for complex neighborhoods on square [18] or SC [19] lattices.

**RESULTS AND DISCUSSION**

**TABLE I.** The critical values of $p_C$ for various neighborhoods based on minimization of $\lambda(p)$ function.

| Neighborhood | $z$ | $p_C$         |
|--------------|----|---------------|
| 4NN          | 6  | 0.3116(12) = pc(NN) |
| 4NN+NN       | 12 | 0.15040(12)   |
| 4NN+2NN      | 18 | 0.15950(12)   |
| 4NN+3NN      | 14 | 0.20490(12)   |
| 4NN+2NN+NN   | 24 | 0.11440(12)   |
| 4NN+3NN+NN   | 20 | 0.11920(12)   |
| 4NN+3NN+2NN  | 26 | 0.11330(12)   |
| 4NN+3NN+2NN+NN | 32 | 0.10000(12) |

For each pair $(p, L)$ of parameters $N_{\text{run}} = 10^4$ lattices with randomly occupied $pL^3$ sites were simulated for $L = 40, 80, 120$ and 160. The wrapping probabilities $W(p, L)$ for various neighborhoods combinations are presented in Fig. 2.

As it was mentioned in the Introduction, the results of computer simulations rather rarely reproduce a single common point of curves $W(p, L)$ unless the number $N_{\text{run}}$ of prepared lattices is very high. It means, that finding the common point of $W(p, L)$ curves for various linear system sizes $L$ may be quite problematic. In order to illustrate better this situation, we plot $W(p, L)$ dependencies near $p_C$ with sites occupation probability step $\Delta p = 10^{-4}$ (see Fig. 3). And indeed, except for 4NN+2NN+NN neighborhood, the curves $W(p, L)$ for various pairs of $L$ intersect at different points. Moreover,
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\[ p_{C}(NN) \approx 0.31160768(15) \] obtained very recently in extensive Monte Carlo simulation [25] and its earlier estimations [26].

Note, however, that reaching such accuracy requires, for \( L \leq 128 \), sampling over \( N_{run} = 5 \cdot 10^{8} \) lattices realization [25], while we recovered the first five digits of \( p_{C}(NN) \) with statistics lower by more than four orders of magnitude.

Knowing percolation threshold may be practically useful for many systems with neighborhoods ranging beyond nearest neighbors [27] or next-nearest neighbors [28]. Thus practical application of \( p_{C} \) values for longer ranges of interaction among systems’ items cannot be generally excluded in all typical applications of the percolation theory, i.e. physics, chemistry, biology and social sciences.

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FIG. 3. (Color online). Wrapping probability \( W(p; L) \) and the pairwise sum \( \lambda(p) \) vs. occupation probability \( p \). The results are averaged over \( N_{\text{run}} = 10^4 \) runs. The symbols (+, ×, *, □) indicate the system linear sizes \( (L = 40, 80, 120, 160) \), respectively. The minima of \( \lambda(p) \) correspond to the percolation thresholds \( p_c \).

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