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

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In this paper, random-site percolation thresholds for a simple cubic (SC) lattice with site 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 $p_C(\text{4NN}) = 0.311\,60(12)$, $p_C(\text{4NN} + \text{NN}) = 0.150\,40(12)$, $p_C(\text{4NN} + \text{2NN}) = 0.159\,50(12)$, $p_C(\text{4NN} + \text{3NN}) = 0.204\,90(12)$, $p_C(\text{4NN} + \text{2NN} + \text{NN}) = 0.114\,40(12)$, $p_C(\text{4NN} + \text{3NN} + \text{NN}) = 0.119\,20(12)$, $p_C(\text{4NN} + \text{3NN} + \text{2NN}) = 0.113\,30(12)$, and $p_C(\text{4NN} + \text{3NN} + \text{2NN} + \text{NN}) = 0.100\,00(12)$, where 3NN, 2NN, and NN stand 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 a lattice constant that is twice as large, the percolation threshold $p_C(\text{4NN})$ is exactly equal to $p_C(\text{NN})$. The simplified method of Bastas *et al.* allows for uncertainty of the percolation threshold value p_C to be reached, similar to that obtained with the classical method but ten times faster.

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I. INTRODUCTION

Finding percolation thresholds p_C and observing cluster properties near a 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 its possible practical applications. The latter ranges from theoretical studies of the geometrical model of the phase transition [6] via condensed-matter physics [7], rheology [8], and forest fires [9], to immunology [10] and quantum mechanics [11].

In the random-site percolation model, the nodes of a 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 that 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 the phase transition as it depends on the linear system size L,

$$X(p;L) = L^{-x}\mathcal{F}\big((p - p_C)L^{1/\nu}\big), \tag{1}$$

where $\mathcal{F}(\cdot)$ is a scaling function, x is a scaling exponent, and ν is a critical exponent associated with the correlation length [1]. Equation (1) yields an efficient way for p_C determination as $L^x X(p_C;L) = \mathcal{F}(0)$ does not depend on the linear system size L. This means that curves $L^x X(p;L)$ 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_{run} of prepared lattices is very high.

Recently, Bastas *et al.* proposed an 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 where curves $X(p;L)$ intercept each other, one may wish to minimize the pairwise difference,

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

with respect to both parameters x and p, where

$$H(p;L) \equiv Y(p;L) \tag{3a}$$

as suggested in Ref. [16] or

$$H(p;L) \equiv Y(p;L) + 1/Y(p;L) \tag{3b}$$

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

$$Y(p;L) \equiv L^x X(p;L). \tag{4}$$

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

In this paper, we propose a simplified version of Bastas *et al.*'s algorithm, where only a single-parameter function $\lambda(p)$ must be minimized in order to provide percolation threshold estimation. With such an 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.

II. APPROACH

Our proposition is to apply Bastas *et al.*'s technique for a quantity such as $X(p;L)$, which does not require scaling along the X axis by a factor L^x in order to achieve statistical invariance of the shape $X(p;L)$ for various values of L. An example of such a quantity is the (top-bottom) wrapping

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probability [20]:

$$W(p;L) = N(p;L)/N_{\text{run}}, \tag{5}$$

where $N(p;L)$ is a number of percolating lattices, with pL^3 occupied sites among N_{run} lattices constructed for fixed values p and L. In the thermodynamic limit, we have $W(p < p_C; L \to \infty) = 0$ and $W(p > p_C, L \to \infty) = 1$, and thus the scaling exponent x of W is equal to zero [1]. Consequently, instead of the form given by Eq. (1), the wrapping probability obeys a simplified scaling relation [1,21],

$$W(p;L) = \mathcal{G}\big((p - p_C)L^{1/\nu}\big). \tag{6}$$

Equation (6) again makes it possible to determine p_C as $W(p_C;L) = \mathcal{G}(0)$ does not depend on the system size L.

Now, the equivalent of Eq. (2) may be written as

$$\lambda(p) \equiv \sum_{i \neq j} \big[H(p;L_i) - H(p;L_j)\big]^2, \tag{7}$$

where

$$H(p;L) \equiv W(p;L) + 1/W(p;L). \tag{8}$$

Following the technique of Bastas *et al.,* one should minimize the function $\lambda(p)$; the found minimum may then be used for the p_C estimation.

Several numerical techniques allow for clusters of connected site identification [21–24]. Here we apply the Hoshen-Kopelman algorithm [22], which allows for sites to be labeled in a such way that occupied sites in the same cluster have assigned the same labels and different clusters have different labels associated with them.

Here we investigate an SC lattice with site neighbors ranging from the nearest neighbors (NN), via the next-nearest neighbors (2NN) and the next-next-next-nearest neighbors (3NN), to the next-next-next-next-nearest neighbors (4NN). A scheme showing only single sites of each of the neighborhood types mentioned above is presented in Fig. 1. The full neighborhoods contain $z = 6$, 12, 8, and 6 sites for NN, 2NN, 3NN, and 4NN neighborhoods, respectively.

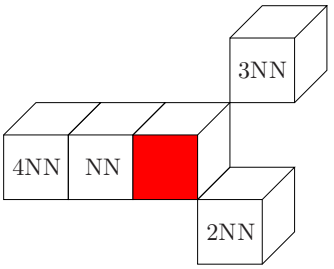

FIG. 1. (Color online) Single sites from various neighborhoods of an SC lattice. The full neighborhoods contain $z = 6$, 12, 8, and 6 sites for NN, 2NN, 3NN, and 4NN neighborhoods, respectively.

Also all available combinations of these neighborhoods are considered, i.e., (4NN+NN), (4NN+2NN), (4NN+3NN), (4NN+2NN+NN), (4NN+3NN+NN), (4NN+3NN+2NN), and (4NN+3NN+2NN+NN) containing $z = 12$, 18, 14, 24, 20, 26, and 32 sites, respectively.

III. RESULTS AND DISCUSSION

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 neighborhood combinations are presented in Fig. 2.

As 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_{run} of prepared lattices is very high. This means that finding the common point of $W(p;L)$ curves for various linear system sizes L may be quite problematic. To better illustrate this situation, we plot $W(p;L)$ dependencies near p_C with a site occupation probability step $\Delta p = 10^{-4}$ (see Fig. 3). And indeed, except for the 4NN+2NN+NN neighborhood, the curves $W(p;L)$ for various pairs of L intersect at different points. Moreover, for the smallest values of L, the dependencies $W(p;L)$ do not even increase monotonically with p. At the same time, the dependencies $\lambda(p;L)$ prepared with the same

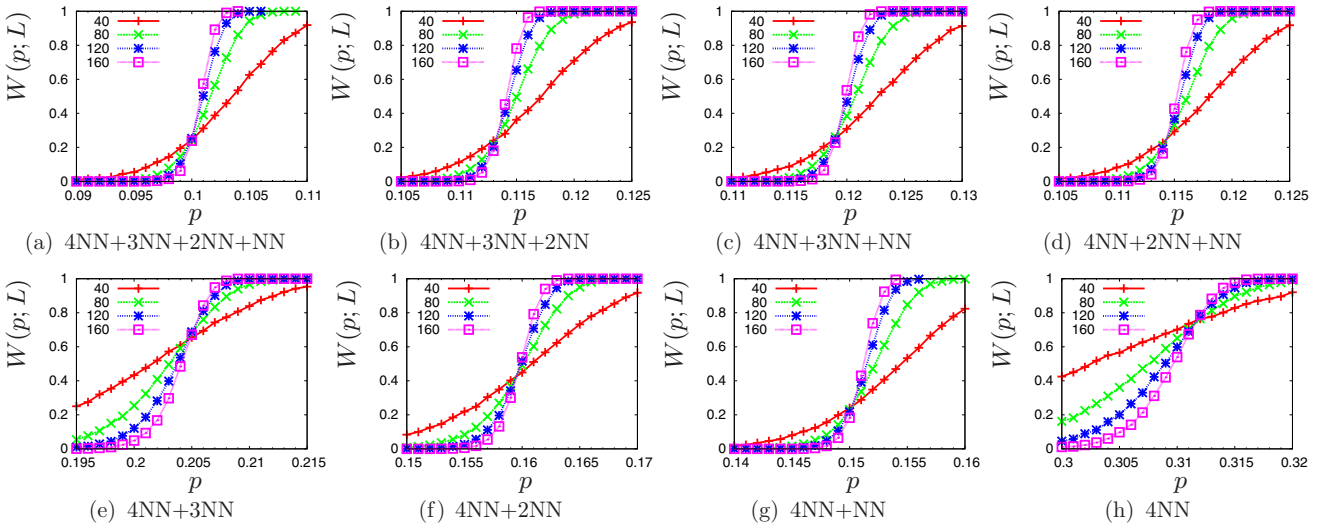

FIG. 2. (Color online) Wrapping probability $W(p;L)$ vs occupation probability p. The results are averaged over $N_{\text{run}} = 10^4$ runs. The symbols (+, ×, ∗ ,□) indicate the system linear sizes ($L = 40$, 80, 120, 160), respectively.

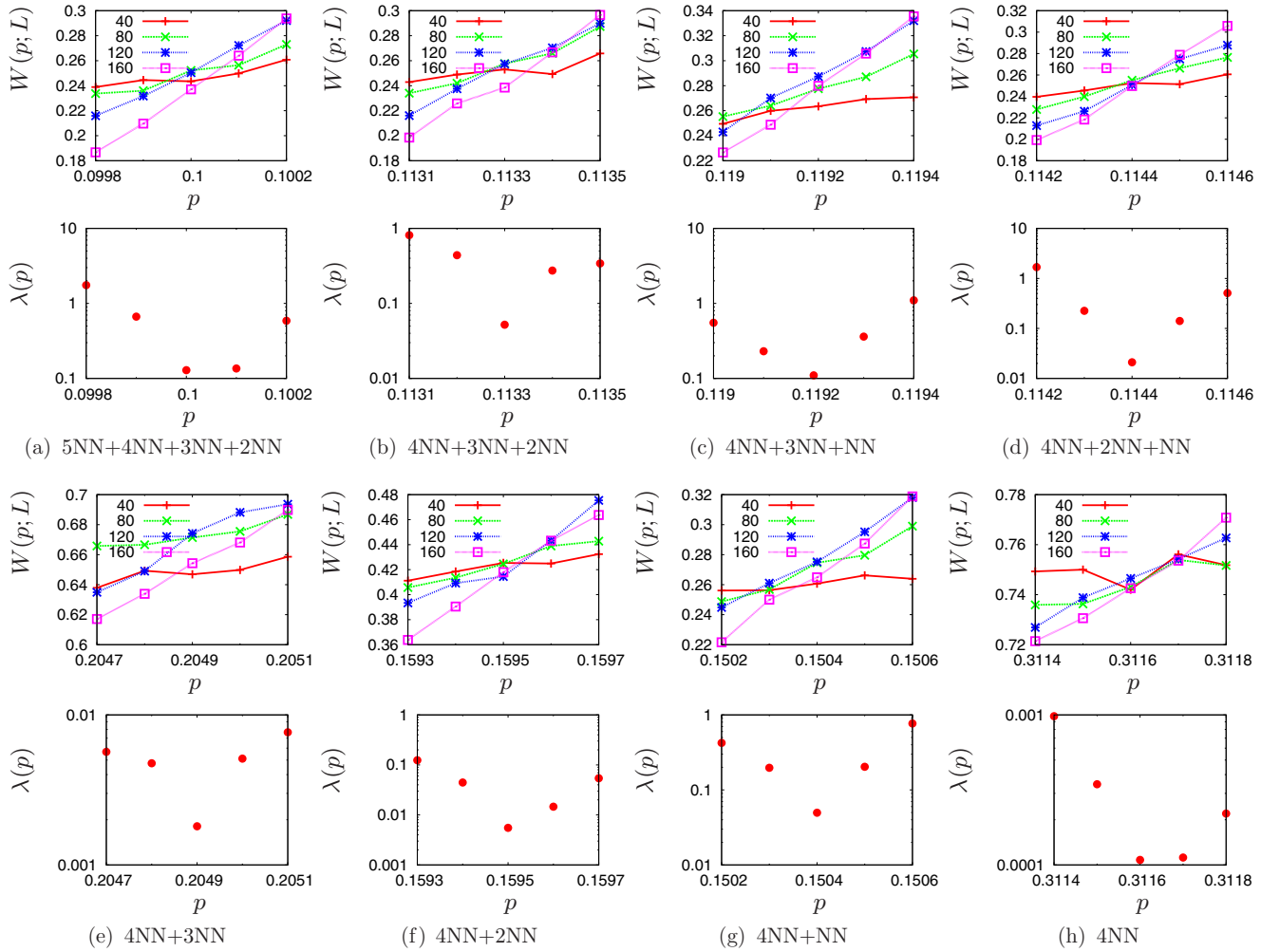

FIG. 3. (Color online) Wrapping probability $W(p;L)$ and the pairwise sum $\lambda(p)$ vs occupation probability p. The results are averaged over $N_{\text{run}} = 10^4$ runs. The symbols (+, × , ∗,□) indicate the system linear sizes ($L = 40$, 80, 120, 160), respectively. The minima of $\lambda(p)$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

accuracy $\Delta p = 10^{-4}$ exhibit a single and sharp minimum (it is worth mentioning that values of λ are presented with the use of a logarithmic scale). The minimum of $\lambda(p)$ corresponds to the percolation threshold p_C. The estimated thresholds are presented in Table I.

The plots $W(p;L)$ presented in Fig. 3 make it possible to determine the length of the interval where the true value of the percolation threshold is located. This length is equal to $\delta_W(p_C) = 0.0004$. Assuming that a real percolation threshold value is uniformly distributed in this interval, one may evaluate the percolation threshold uncertainty as $u_W(p_C) = \delta_W(p_C)/\sqrt{3} \approx 0.000\,23$. The approach based on the $\lambda(p;L)$ dependence provides an evaluation of $\delta_\lambda(p_C)$ that is twice as small, and consequently $u_\lambda(p_C) \approx 0.000\,12$. On the other hand, the method of p_C estimation based solely on $W(p;L)$ dependences, applied for similar neighborhood geometries, leads to twice as small lengths $\delta(p_C)$ and consequently similar uncertainties $u(p_C)$ but for ten times larger sampling ($N_{\text{run}} = 10^5$) [19]. One can conclude that the method used by Bastas *et al.* leads to uncertainty of the percolation threshold value p_C similar to that obtained with the classical method $u_\lambda(p_C) \approx u_W(p_C)$, but ten times faster.

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

Neighborhood	z	p_C
4NN	6	$0.31160(12) = p_C(\text{NN})$
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)

Note that an SC lattice with 4NN neighbors may be mapped onto two independent interpenetrated SC lattices but with a lattice constant that is twice as large. Thus we expect the percolation threshold p_C(4NN) for the next-next-next-next-nearest neighbors to be equal exactly to p_C(NN). Indeed, the obtained value of $p_C(4\text{NN}) \approx 0.31160$ agrees very well with values of the percolation threshold estimated for the

nearest neighbors $p_C(\mathrm{NN}) \approx 0.311\,607\,68(15)$ obtained very recently in extensive Monte Carlo simulation [25] and its earlier estimations [26].

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

Knowing the 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 the 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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