Journal of Statistical Physics, Vol. 82, Nos. 3/4, 1996

Histogram Monte Carlo Position-Space Renormalization Group: Applications to the Site Percolation

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Received January 31, 1994; final June 16, 1995

We study site percolation on the square lattice and show that, when augmented with histogram Monte Carlo simulations for large lattices, the cell-to-cell renormalization group approach can be used to determine the critical probability accurately. Unlike the cell-to-site method and an alternate renormalization group approach proposed recently by Sahimi and Rassamdana, both of which rely on *ab initio* numerical inputs, the cell-to-cell scheme is free of prior knowledge and thus can be applied more widely.

KEY WORDS: Percolation; renormalization group; Monte Carlo; critical point.

1. INTRODUCTION

The problem of percolation has been a subject of much contention in recent years.[1,2] Percolation has been investigated using a variety of approaches, including series expansions,[3] Monte Carlo simulations,[4-7] position-space renormalization group analyses,[8,9] histogram Monte Carlo renormalization group studies,[10-15] and conformal invariance analyses.[16] In most of these investigations one invariably considers the evaluation of $E(L, p)$, the existence probability[11-15] that the system percolates, as a function of L, the linear dimension of the lattice, and p, the site (or bond) occupation probability. The existence probability has also been termed the crossing probability by Kesten[1] and the spanning probability by Ziff.[6] In the limit of $L \to \infty$, $E(L, p)$ approaches a step function $\theta(p - p_c)$,[2] where p_c is the critical probability. For the square lattice with free boundary

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0022-4715/96/0200-1199$09.50/0

conditions, $E(\infty, p_c)$ is given by a universal constant $\alpha_c = 1/2$ for both bond and site percolation.[6]

Consider the determination of p_c for site percolation on the square lattice. Although early attempts using series expansion[3] yielded the value $p_c = 0.593 \pm 0.02$, the best value to date is that of Ziff[6], who used extensive Monte Carlo simulations to arrive at $p_c = 0.592\,7460 \pm 0.000\,0005$. In addition, the scaling behavior of p_c has been found to assume the form

$$p_c(L) - p_c \sim L^{-1/\nu} \tag{1}$$

under a cell-to-site renormalization group scheme,[8, 9] where $\nu = 4/3$ is the correlation exponent, and $p_c(L)$ is the fixed point solved from the transformation equation

$$p_c(L) = E[L, p_c(L)] \qquad \text{(cell-to-site)} \tag{2}$$

Similarly, under a cell-to-cell renormalization group scheme, the scaling behavior is found to be[6]

$$p_c(L) - p_c \sim L^{-1-1/\nu} \tag{3}$$

with $p_c(L)$ solved from

$$E[L-1, p_c(L)] = E[L, p_c(L)] \tag{4}$$

In addition, Ziff[6] has proposed an alternate approach based on the scaling relation (3) and the solution of the equation

$$E[L, p_c(L)] = \alpha \tag{5}$$

where the value of $\alpha = \alpha_c = 0.5$ was used. Very recently, Sahimi and Rassamdana (SR)[17] showed that the usefulness of (5) can be extended to any value of $0 < \alpha < 1$. For this reason we shall refer to (5) in the context of general α as the SR equation. In discussions in refs. 6 and 17, however, the primary purpose was the determination of the scaling behavior using data for relatively small values of $L \leqslant 7$. It is also necessary in their analyses that specific values of the exponents are to be used.

The purpose of this paper is twofold. First, we carry out a cell-to-cell renormalization group scheme proposed recently by one of us[13] for large lattices with $L \leqslant 512$, a process made possible by using histogram Monte Carlo simulations. Second, we show that the cell-to-cell scheme is fundamentally more useful. Using the same Monte Carlo data, we show that the cell-to-cell approach determines p_c accurately, and that the determination is independent of the value of the scaling exponent used in the

extrapolation. Thus, the cell-to-cell approach is more useful and capable of a wider range of applications.

2. HISTOGRAM MONTE CARLO SIMULATIONS

The histogram Monte Carlo renormalization approach[11] to site percolations has been described in recent papers.[13–15] Here, for completeness and to make our presentation self-contained, we briefly sketch the main ideas. Consider site percolation on a lattice G of N sites, with each site either occupied with a probability p or empty with a probability $1-p$. Two neighboring sites belong to a cluster if both are occupied. The occupied sites form subgraphs $G' \subset G$ consisting of clusters of sites. Let $v(G')$ be the number of occupied sites in G'. The probability of the appearance of a particular subgraph G' is

$$\pi(G', p) = p^{v(G')}(1-p)^{N-v(G')}, \qquad 0 \leqslant v(G') \leqslant N \tag{6}$$

A cluster is percolating if it spans across opposite borders of G. A percolating subgraph, denoted by G'_{per}, is one whose largest cluster is percolating. The existence probability $E(L, p)$ for site percolation on a square lattice G of size $L \times L$ with free boundaries is then the summation of the probability (6) over all percolating clusters, namely,

$$E(L, p) = \sum_{G'_{\text{per}} \subseteq G} \pi(G'_{\text{per}}, p) = \sum_{v=0}^{N} p^v (1-p)^{1-v} M(v) \tag{7}$$

where $M(v)$ is the number of percolating subgraphs of G for a fixed v. This latter expression permits one to evaluate the existence probability $E(L, p)$ numerically.

We evaluate (7) by computing $M(v)$ from histogram Monte Carlo simulations. One first chooses w distinct p values, and for each of the p values generates N_R subgraphs at random. For each of the wN_R subgraphs thus generated, one counts v, the number of occupied sites, and checks whether the subgraph is percolating. In this way, one obtains $N_{\text{per}}(v)$, the number of percolating subgraphs, and $N_{\text{np}}(v)$, the number of nonpercolating subgraphs, for each given v. The central idea of ref. 13 is to approximate $M(v)/\binom{N}{v}$, the actual fraction of subgraphs that are percolating, by $N_{\text{per}}(v)/[N_{\text{per}}(v) + N_{np}(v)]$, the fraction of subgraphs that are percolating in the wN_R subgraphs generated in the simulations. Then (7) becomes

$$E(L, p) \approx \sum_{v=0}^{N} p^v (1-p)^{N-v} \binom{N}{v} \left[\frac{N_{\text{per}}(v)}{N_{\text{per}}(v) + N_{\text{np}}(v)} \right] \tag{8}$$

This equation forms the basis of our numerical analysis.

3. THREE DIFFERENT CALCULATION SCHEMES AND NUMERICAL ANALYSES

We use the cell-to-cell renormalization group transformation[11,12]

$$E(L/2, p') = E(L, p) \tag{9}$$

connecting two cells of linear sizes L and $L/2$. This transformation gives the renormalized occupation probability p' as a function of p. The fixed point $p_c(L)$ of (9), obtained by solving the equation

$$E[L/2, p_c(L)] = E[L, p_c(L)] \qquad \text{(cell-to-cell)} \tag{10}$$

gives an estimate of the critical probability $p_c(L)$ for each value of L.

We have carried out histogram Monte Carlo simulations as described in Section 2 with $w \sim 400$ and $N_R \sim 10^5$–10^6 for systems of sizes $L =$ 32, 64, 128, 256, and 512. The data are then applied to calculate $p_c(L)$ using the three calculations schemes described by (10), (2), and (5), namely the cell-to-cell, cell-to-site and SR approaches. Results obtained from (10) and (2) are listed in Table I, and results from (5) are listed in Table II for three different values of $\alpha = 0.1, 0.5$, and 0.9. These results are further plotted in Figs. 1–3 by assuming the scaling behavior

$$p_c - p_c(L) \sim L^{-c} \tag{11}$$

for $c = 0.75$, 1.00, and 1.75. The value of $p_c = p_c(\infty)$ is then extrapolated by least-square fits in each of the cases. Results are shown in Table III.

Table III show clearly that, among the three schemes, the cell-to-cell scheme leads to the most accurate determination of p_c. More importantly, numbers in the first line of Table III show that the determination of p_c using the cell-to-cell scheme is *insensitive* to the value of the scaling power c in the scaling relation (11). This is due to the relatively large values of L

Table I. Values of $p_c(L)$ Under the Cell-to-Cell and Cell-to-Site Schemes[a]

L	Cell-to-cell	Cell-to-site
32	0.59287 ± 0.00054	0.60257 ± 0.00019
64	0.59288 ± 0.00030	0.59845 ± 0.00007
128	0.59273 ± 0.00018	0.59607 ± 0.00006
256	0.59291 ± 0.00024	0.59476 ± 0.00008
512	0.59283 ± 0.00014	0.59397 ± 0.00005

[a] Numbers for cell-to-cell are solved from (10) and cell-to-site from (2).

Table II. Values of $p_c(L)$ Under the SR Scheme Solved from (5)

L	$\alpha = 0.1$	$\alpha = 0.5$	$\alpha = 0.9$
32	0.54217 ± 0.00019	0.59264 ± 0.00017	0.64138 ± 0.00017
64	0.56263 ± 0.00010	0.59273 ± 0.00007	0.62215 ± 0.00008
128	0.57484 ± 0.00011	0.59273 ± 0.00006	0.61040 ± 0.00007
256	0.58219 ± 0.00009	0.59280 ± 0.00009	0.60336 ± 0.00005
512	0.58648 ± 0.00008	0.59280 ± 0.00007	0.59910 ± 0.00006

used in the extrapolation. In contrast, numbers in the second line from the cell-to-site scheme indicate that it works well only when one takes $c = 1/\nu = 0.75$, and the last three lines indicate that the SR scheme works well only when α is taken to assume the critical value $\alpha_c = 0.5$. Thus, both of the latter approaches rely on some form of *ab initio* input.

These situations are also illustrated in Figs. 1–3. In Fig. 1, where one takes $c = 1/\nu = 0.75$, it is seen that all three schemes work almost equally well, and in Figs. 2 and 3, where $c = 1.0$ and 1.75, respectively, it is seen that only the cell-to-cell scheme and the SR scheme with the special input value of $\alpha = 0.5$ yield good results.

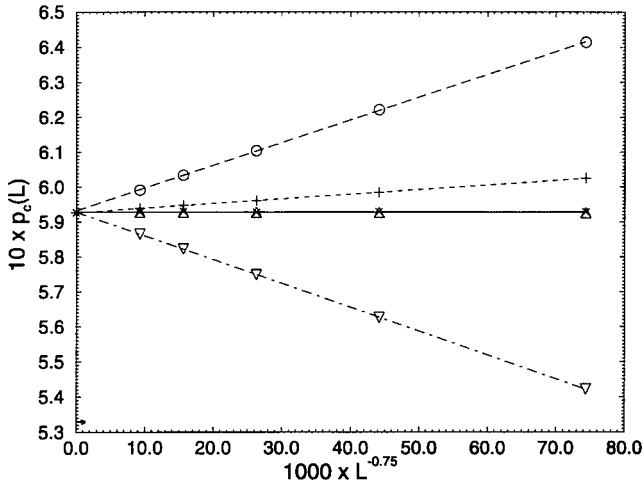

Fig. 1. Plot of $p_c(L)$ as a function of $L^{-0.75}$. Data points are those obtained using the cell-to-cell scheme ($\times$), the cell-to-site scheme ($+$), and the SR scheme ($\triangle$, $\alpha = 0.5$; ∇, $\alpha = 0.1$; $\bigcirc$, $\alpha = 0.9$). The star ($*$) indicates the value $p_c = 0.592746$ determined by Ziff.[6] Straight lines represent least square fits, and intersections of the straight lines with the y axis give the values of p_c listed in Table III.

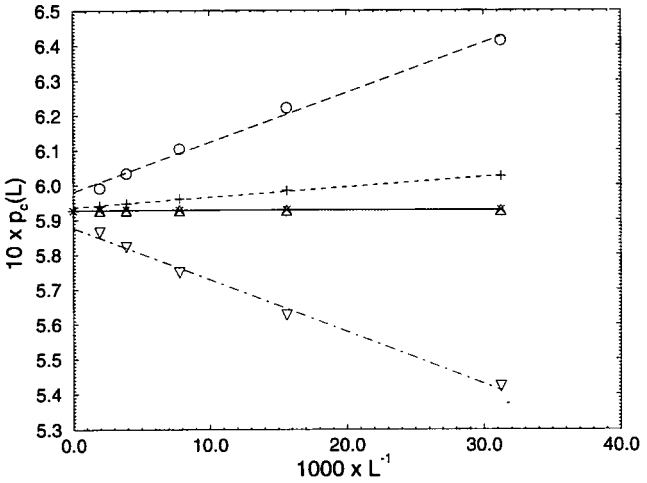

Fig. 2. Plot of $p_c(L)$ as a function of $L^{-1.00}$. Data points and notations are the same as those in Fig. 1.

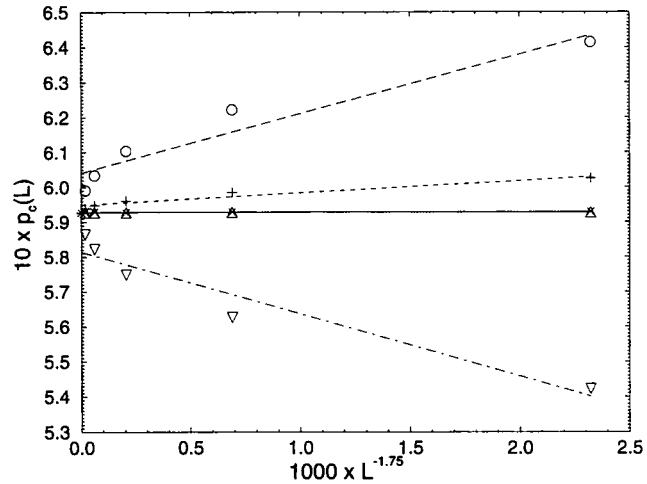

Fig. 3. Plot of $p_c(L)$ as a function of $L^{-1.75}$. Data points and notations are the same as those in Fig. 1.

Table III. The Critical Probability p_c Extrapolated from Data of Tables I and II by Assuming the Scaling Relation L^{-c}

c	0.75	1.00	1.75
Cell-to-cell	0.59282 ± 0.00006	0.59283 ± 0.00005	0.59283 ± 0.00004
Cell-to-site	0.59267 ± 0.00006	0.59364 ± 0.00016	0.5949 ± 0.0005
SR, $\alpha = 0.1$	0.59279 ± 0.00004	0.58772 ± 0.00115	0.5814 ± 0.0030
SR, $\alpha = 0.5$	0.59283 ± 0.00002	0.59281 ± 0.00002	0.59278 ± 0.00002
SR, $\alpha = 0.9$	0.59322 ± 0.00014	0.59807 ± 0.00120	0.6041 ± 0.0030

4. CONCLUSION AND DISCUSSION

We have considered the site percolation problem on the square lattice using the cell-to-cell renormalization group schemes, as well as an alternate scheme proposed by Ziff and extended recently by Sahimi and Rassamdana (SR). The transformation relation determing $p_c(L)$ is solved in each case using data from histogram Monte Carlo simulations for cells of size $L \times L$, with $L = 2^l$, $l = 5, 6, ..., 9$. The results are then used to extrapolate the critical probability p_c. Our results show that all three schemes can be used to determine p_c with almost the same degree of accuracy. However, the cell-to-site scheme makes use of the prior knowledge of the exponent $-1/\nu = -3/4$ of the scaling relation, and the SR scheme, while of a lesser dependence on the exponent used, requires the use of the universal constant $\alpha_c = 1/2$ in the determining equation. The cell-to-cell scheme, in contrast, does not require any *ab initio* input.

Finally, we remark that, being insensitive to the scaling power used in the extrapolation of p_c, the present cell-to-cell scheme, which works well for systems with relatively large L, does not settle a recent controversy on the precise value of the scaling power.[18, 19] Instead, the present scheme's usefulness rests on precisely this insensitivity so that it can be applied to other systems when the scaling power is not known.

ACKNOWLEDGMENTS

One of us (C.K.H.) would like to thank D. Stauffer for calling his attention to ref. 17 and M. Sahimi for useful discussions. We are also indebted to H. Gould for a critical reading of the manuscript and the referees for valuable comments. The work by C.K.H. is supported by the National Science Council of the Republic of China (Taiwan) under grant numbers NSC 84-2112-M-001-013 Y and 84-0501-I-001-037-B12; he also acknowledges the Department of Physics at Northeastern University and

that at Harvard University for providing research facilities. The work by F.Y.W. is supported by the National Science Foundation through grants DMR-9313648 and INT-9207261.

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Communicated by D. Stauffer