LETTER TO THE EDITOR

Site percolation threshold for square lattice

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Abstract. In order to find out as precisely as possible the site percolation threshold in the square lattice, a Fortran high speed Monte Carlo program has been developed (2.2–2.4 μs per site on CDC Cyber 76) for simulating site percolation in $L \times L$ square lattice with $L = 50$ to 50 000. Using $L = 750$ to 16 000 we found $p_c = 0.592\,77 \pm 0.000\,05$. This value is within the confidence limits of values published earlier ($p_c = 0.5931 \pm 0.0006$, $p_c = 0.5923 \pm 0.0007$ and $p_c = 0.5927 \pm 0.0002$). Three test checks with $L = 50\,000$ confirmed this result within the above error bars.

Whereas percolation thresholds p_c for triangular site percolation, triangular bond percolation, honeycomb bond percolation and square bond percolation are known, there are no exact solutions for the site percolation threshold in the square lattice so far. The latest values previously approximated by different methods,

Monte Carlo	0.5931 ± 0.0006	(Reynolds *et al* 1980),
Transfer matrix	0.5927 ± 0.0002	(Derrida and de Seze 1982),
Series expansion	0.5923 ± 0.0007	(Djordjevic *et al* 1982)

show agreement within error bars. A more accurate percolation threshold in the square lattice enables us to check if the above methods and their estimated errors are reliable. We will find that the values for the site percolation threshold p_c in the square lattice outside the range

$$0.5928 \pm 0.0001$$

appear unlikely.

The Monte Carlo method we used to ascertain p_c is very similar to the method used by Reynolds *et al* (1980). We reduced a three-dimensional percolation program as explained by Stauffer (1981) to two dimensions and optimised the computing time. The essential steps of this optimisation are outlined in the following.

First we integrated the sub-program (LASS) into the main program. Then we consequently broke up the five possible branches depending on the occupation status of their neighbours. Also, the identical passages within the branches were programmed repeatedly. We attached great importance to obtaining each branch with a minimum of if-statements. We omitted all unnecessary variables. The percolation program thus obtained analysed square lattices with a speed of 2.2 μs per site. For the determination of p by iteration we applied a procedure similar to that explained by Eschbach (1980)

$$\Delta = DL^{-0.75}$$

where $D = 0.35$. Δ is the initial step by which we change the trial value for p_c (Reynolds *et al* 1980). 0.75 is the presumably exact (Stauffer 1981) reciprocal correlation length exponent.

The accuracy with which p_c is determined for one set of random numbers is obtained by

$$\Delta 2^{-i}, \qquad i = \text{number of iterations.}$$

As there is only a limited computing time, $T(L)$, available for the size L of each system, the number i of iterations decreases with the number N of different sequences of random numbers used

$$(3 + i)N \propto T(L).$$

The factor 3 is required because on the average we need three checks, whether top and bottom are connected, before p_c is iterated. The number N of realisations determines the statistical error, apart from a factor A:

$$\text{statistical error} = AN^{-1/2}$$

with $A = 0.5 \, L^{-0.75}$, where $1/0.75$ again is the correlation length exponent. The factor 0.5 was estimated empirically.

We minimised the total squared error

$$(\Delta 2^{-i})^2 + (AN^{-1/2})^2$$

and obtained

$$i = (\ln(\text{constant } T(L))/\ln(4).$$

Table 1 shows that the number of iterations needed according to this relation was exceeded in most cases. The greater accuracy so obtained justifies neglecting the error due to the limited number of iterations for one sequence of random numbers.

With the program explained so far systems with $L = 50$ to 400 were calculated. For processing larger systems an improved version of recycling, which reduces the memory required by the Hoshen–Kopelman (1976) algorithm, was applied (Margolina *et al* 1983). The average computing time per site for $L = 1000$ to 16 000 was about 3% longer than the previous time only (2.2 μs per site). Whereas for $L = 1000$ in general only one recycling per cluster check was needed, $L = 16\,000$ required about 700 recyclings, which means that the memory sites had to be recycled after the analysis of 16 rows on the average. The total computing time $L = 50$ to 16 000 was only $18\frac{1}{2}$ hours.

Only with $L = 50\,000$ the computing time was increased by about 11% to 2.45 μs per site. Our total computing time for $L = 50\,000$, with which checked for systematic size effects in our extrapolation, was $14\frac{1}{2}$ hours. The values are shown in table 1 and figure 1.

In order to extrapolate p_c we took the values $\langle p \rangle$ for $L = 50$ to 16 000 from table 1 (including the values marked R from Reynolds *et al* (1980)). First we subtracted the finite-size trend from each value and calculated the weighted average

$$p_c = 0.592\,77 \pm 0.000\,04.$$

Instead, with weighted linear regression line we obtained

$$p_c = 0.592\,78 \pm 0.000\,05.$$

Table 1. Monte Carlo results for site percolation in square lattices. Values marked R are taken from Reynolds *et al* (1980). The statistical error s was calculated from $s = [\sigma/(N-1)]^{1/2}$, N being the number of realisations and $\sigma^2 = \langle p^2 \rangle - \langle p \rangle^2$.

| L	No of realisations	$\langle p \rangle$	s	No. of iterations
50	11 000	0.592 33	0.000 27	9
64 R	6 495	0.592 6	0.000 29	
100 (R)	4 080	0.592 28	0.000 26	(9)
150 R	1 725	0.592 7	0.000 30	
200 R	1 005	0.592 0	0.000 30	
300	1 000	0.592 37	0.000 23	9
400	1 000	0.592 86	0.000 19	9
500 R	1 005	0.592 6	0.000 16	
750	700	0.592 74	0.000 13	7
1000	450	0.592 74	0.000 14	7
2000	100	0.592 91	0.000 19	7
4000	25	0.592 89	0.000 18	7
8000	21	0.592 77	0.000 09	7
16000	3	0.592 65	0.000 20	7
50000 a	1	0.592 88		2
50000 b	1	0.592 54		1
50000 c	1	0.592 65		1
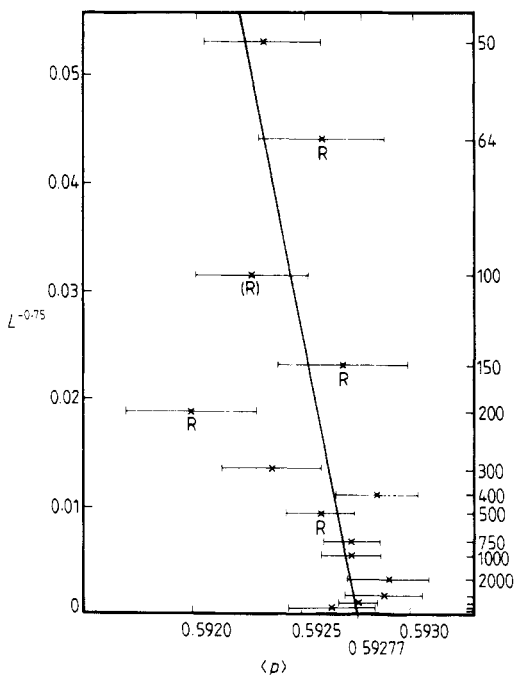
Figure 1. Extrapolation of site percolation threshold for square lattices, analogous to Reynolds *et al* (1980). The weighted regression straight line is shown. Values found by Reynolds *et al* (1980) are marked R. The significant stabilisation of $\langle p \rangle$ for $L = 750$ to 16 000 should be noted.

In figure 1 this weighted regression line is shown. From there

$$p_c = 0.592\,80 \pm 0.000\,10$$

for $L \to \infty$ can be extrapolated also visually.

By summing up the three results for $L = 50\,000$ we obtained a value of

$$0.592\,70 \pm 0.000\,10.$$

Summarising all four results we estimated

$$p_c = 0.592\,77 \pm 0.000\,05.$$

A determination of p_c from $L = 50\,000$ alone, with an accuracy $\pm 0.000\,05$ as obtained by extrapolation of the results of $L = 50$ to $16\,000$, would require a computing time of about 45 hours, using nine realisations. Although we could have used systems beyond $L = 50\,000$, we did not do so since computing times would have been too long. For more numerical details see Gebele (1983).

If the p_c values so obtained are compared with the published results of other methods as mentioned before, these latter methods and their error estimates are confirmed. There is a particularly good consistence with the value 0.5927 ± 0.0002 calculated through the transfer matrix by Derrida and de Seze (1982).

We conclude: at present Monte Carlo simulation presents the most accurate results for p_c. However, the larger error bars found by other methods were show to be realisitc. Our value would be useful for future speculations about the exact value for this percolation threshold.

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