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Spreading of percolation in three and four dimensions

Peter Grassberger

Physics Department, University of Wuppertal, D-56 Wuppertal 1, Gauss-Strasse 20, West Germany

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Abstract. We present Monte Carlo simulations of the spreading of bond percolation on three- and four-dimensional simple (hyper-)cubic lattices. The algorithm is the same as that applied previously in two dimensions, with the spreading proceeding from a hyperplane. We find the spreading dimension to be $\hat{d} = 1.82 \pm 0.02$ (three-dimensional) and $\hat{d} = 1.88 \pm 0.03$ (four-dimensional). Also, we obtain values of the percolation probability and of the static exponents with errors at least comparable to the best values from the literature.

Recently, much interest has been devoted to one particular way of growing large percolation clusters. The method starts from some seed, incorporates in a first step all sites connected to it by unbroken bonds, and then proceeds to the next step. The sites connected to the seed by t unbroken bonds are called 'growth sites' at the tth step, since it is through them that the cluster grows in this step (Middlemiss *et al* 1980, Alexandrowicz 1980, Pike and Stanley 1981, Grassberger 1983, 1985, Hong and Stanley 1983a, b, Rammal *et al* 1984, Havlin and Nossal 1984, Herrmann *et al* 1984, Vannimenus *et al* 1984). Actually, this description applies to bond percolation. Bond percolation is considered throughout this paper; the formulation for site percolation is analogous.

Physical realisations of this type of growth are the spreading of forest fires or epidemics (Grassberger 1983). In the latter context it is called the 'general epidemic process' (Bailey 1975).

While the main interest in this process is its time behaviour, it appears that it is also one of the most convenient methods to study ordinary percolation by Monte Carlo techniques. The latter is obtained at the limit $t \to \infty$.

In all papers except those by Grassberger, the seed was taken to be a single site. In contrast, in Grassberger (1983, 1985) two-dimensional percolation was studied by taking an infinitely long line as the seed. The main advantage is that one has large 'clusters' from the very beginning, so that the fluctuations are small. When starting from a single site, one has very large fluctuations provided the clusters are still small. Also, small lattices can be used more efficiently, and distances from the seed are computed more easily.

In the present paper, we shall present results from Monte Carlo simulations in three and four dimensions. We closely follow Grassberger (1985), to which we refer for details of the algorithm. We take as seeds the hyperplanes $x = 0$. Spreading then proceeds perpendicular to them into the positive x direction. In three dimensions, we used lattices of size $120 \times 128 \times 128$, with periodic boundary conditions at the sides. Spreading always stopped before the far boundary ($x = 120$) was reached. This modest

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size was dictated by the small core memory available (60 000 words of 60 bits). In four dimensions, we used a bigger computer, allowing us to run lattices of size $60\times48\times48\times48$. To obtain the correct critical value of p, we made runs at nine different values of p for $d=3$. For every value of p, we made 500–1600 independent runs with about 320 time steps each, corresponding to a total number of about 10^9 wetted sites. For $d=4$, we made about 500–800 runs with up to 200 time steps at eleven different values of p, leading to $\sim1.2\times10^9$ wetted sites.

The measured quantities were the average number N_t of the growth sites in the tth step and their average x_t (i.e. their average distance from the seed). Results for $d=3$ are shown in figures 1 and 2.

At the critical point we expect that

$$\langle x_t\rangle \sim t^{z_1} \tag{1}$$

and

$$N_t \sim t^{-z_2}. \tag{2}$$

Notice that z_1 is called $1/z$ in Janssen (1985), $\tilde{\nu}$ in Havlin and Nossal (1984), $d_{\min}$ in Stanley (1984), ν_t in Alexandrowicz (1980) and ψ_{23} in Pike and Stanley (1981).

Equations (1) and (2) should of course only hold for infinite lattices. Due to the finite width of the lattice, we have corrections whose signs can fortunately be estimated; since the number of growth sites ultimately has to decay exponentially on a finite lattice, the finite-size corrections tend to enhance the effective exponent z_2. Similarly, since the distance $\langle x_t\rangle$ has to grow linearly (once it is much larger than the transverse

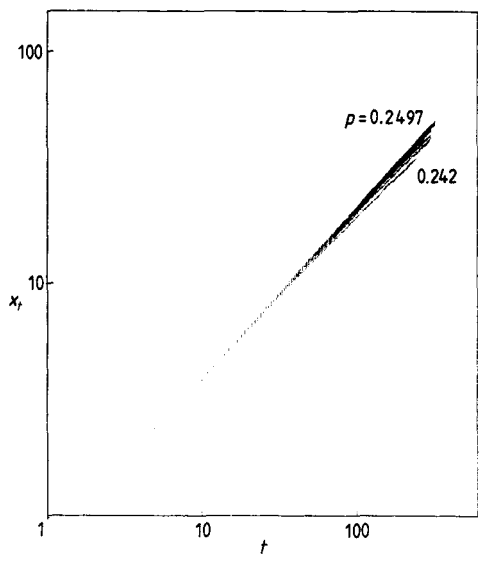

Figure 1. Average distance x_t of growth sites from the starting surface for bond percolation in three dimensions plotted against time t on a doubly logarithmic scale for different values of p (these values are the same as in figure 2).

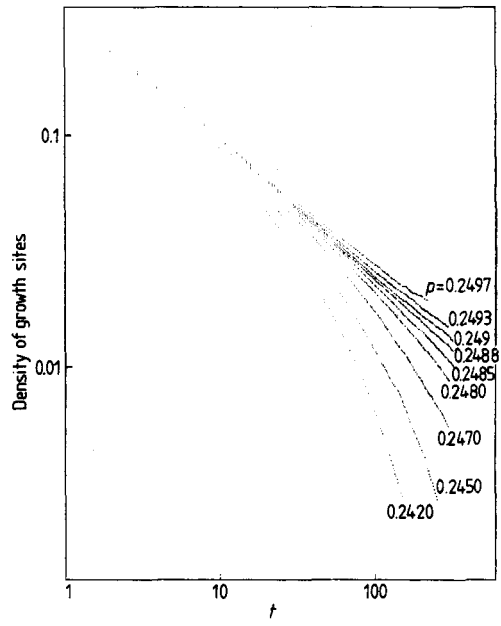

Figure 2. Density of growth sites (absolute number N_t divided by starting surface) for bond percolation in three dimensions, plotted against time t on a doubly logarithmic scale for different values of p.

width), the effective exponent z_1 is also overestimated. An error in p_c has, in contrast, opposite effects on estimates of z_1 and z_2. Thus finite-size corrections cannot be confused with errors in p_c. Another test for finite-size corrections consists of performing runs on much smaller lattices. We have done this, and conclude that these corrections are completely negligible.

Values of p_c and of the exponents z_i could be read directly from figures 1 and 2. Due to possible corrections to scaling, we considered this to be unsatisfactory. Instead, we show in figures 3 and 4 effective exponents obtained by fitting equations (1) and (2) to intervals $[t/4, t]$ for all t. The correct exponents are equal to the limits for $1/t \to 0$. We see in figure 3 that straight extrapolations in $1/t$ are not possible for any value of p, showing that there are indeed non-negligible corrections to scaling. On the other hand, such an extrapolation is possible in figure 4, yielding

$$\left.\begin{aligned} p_c &= 0.248\,65 \pm 0.000\,13 \\ z_2 &= 0.63 \pm 0.02 \end{aligned}\right\} \quad (d=3). \tag{3, 4}$$

Using this value of p_c then gave

$$z_1 = 0.725 \pm 0.006 \qquad (d=3) \tag{5}$$

and gave the correction-to-scaling exponent Δ, defined by

$$\langle x_t \rangle = t^{z_1}(1 + a/t + bt^{-\Delta}) \tag{6}$$

as $\Delta = 0.65 \pm 0.1$.

The data for $\langle x_t \rangle$ and N_t in four dimensions are shown in figures 5(a) and 6(a). When effective slopes are fitted to them in the same way they give the results shown in figures 5(b) and 6(b). Again we see that no linear fit is possible to the slopes of

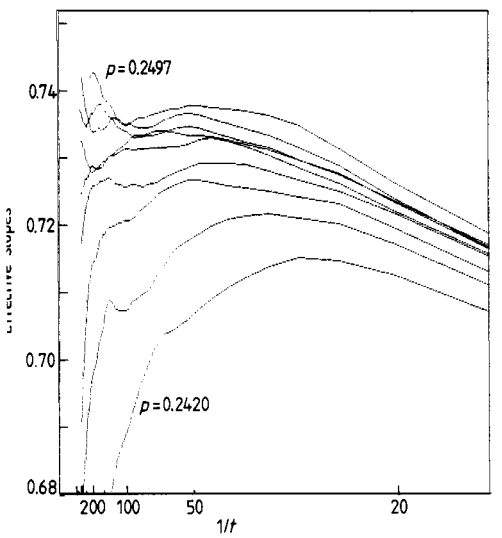

Figure 3. Average slopes of figure 1, averaged over the last $\frac{3}{4}$ of the time steps, and plotted against $1/t$. At the critical point, this slope should depend linearly on $1/t$ if there are no corrections to scaling with exponent <1. The extrapolation to $1/t \to 0$ gives z_1, for $p = p_c$.

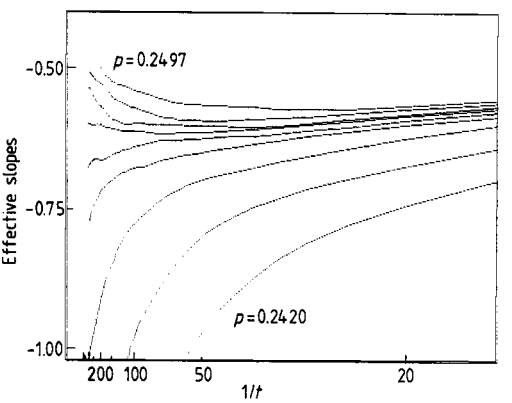

Figure 4. Same as figure 3, but for the data of figure 2. The extrapolation to $1/t \to 0$ gives $-z_2$.

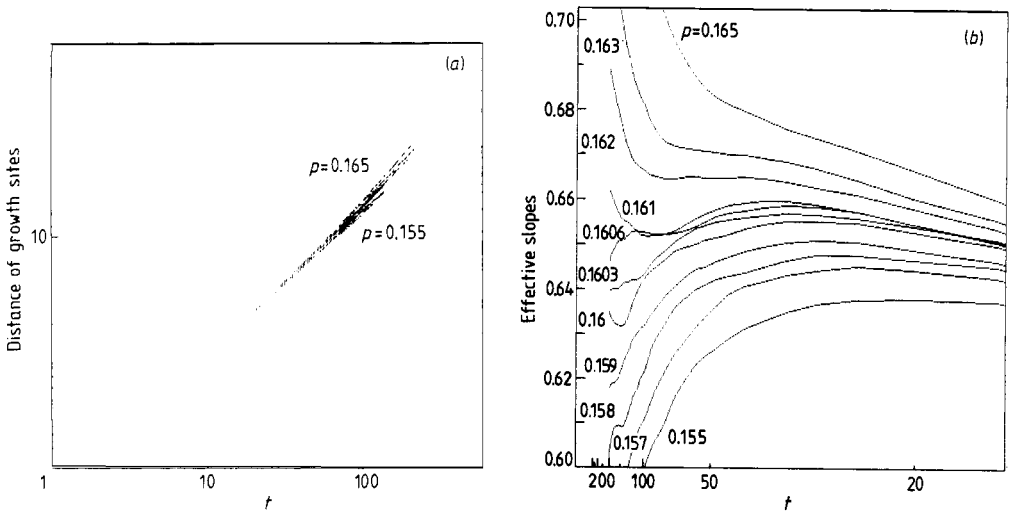

Figure 5. (*a*) Same as figure 1, but for four dimensions. The values of p are given in figure 5(*b*). (*b*) Same as figure 3, but for four dimensions.

$\langle x_t \rangle$, suggesting a correction-to-scaling exponent $\Delta = 0.65 \pm 0.2$. Proceeding further, as in the three-dimensional case, we are led to

$$\left.\begin{aligned} p_c &= 0.160\,13 \pm 0.000\,12 \\ z_1 &= 0.615 \pm 0.010 \\ z_2 &= 0.97 \pm 0.03 \end{aligned}\right\} \qquad (d=4). \tag{7, 8, 9}$$

Away from the critical point, we have the scaling ansatz for the density $\rho(x, t)$ of growth sites (Grassberger 1983)

$$\rho(x, t) \simeq t^{-[(\beta/\nu_t)+1]} F(\varepsilon x^{1/\nu}, \varepsilon t^{1/\nu_t}) \qquad \varepsilon = p - p_c \tag{10}$$

from which we obtain z_1 and z_2 in terms of the static exponents β and ν, and of a kinetic exponent ν_t (which was called τ in Alexandrowicz (1981) and Grassberger (1983), $\nu_\parallel$ in Grassberger (1985) and $\xi_{\min}$ in Hong and Stanley (1983a, b)):

$$z_1 = \nu/\nu_t \tag{11}$$

$$z_2 = 1 - [(\nu - \beta)/\nu_t]. \tag{12}$$

This ansatz implies the usual (hyper-)scaling relations. From the above we can already obtain the ratio β/ν, or equivalently the exponent

$$\eta = \frac{2\beta}{\nu} - d + 2 = \begin{cases} -0.02 \pm 0.04 & (d=3) \\ -0.10 \pm 0.09 & (d=4). \end{cases} \tag{13}$$

Further exponents can be derived by standard scaling relations. They include the fractal dimension d_F of the infinite cluster at p_c, and the spreading dimension $\hat{d}$ (defined via the number M_T of growth sites with $t < T$ in the infinite cluster, when grown from a single-site seed, as $M_T \sim T^{\hat{d}}$; it is called the 'chemical distance dimension' d_l in

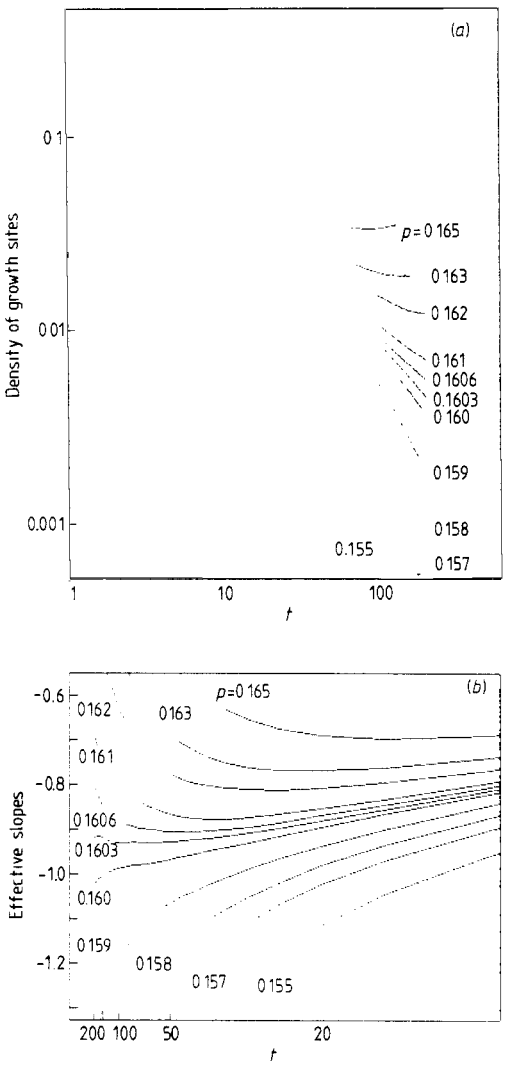

Figure 6. (*a*) Same as figure 2, but for four dimensions. (*b*) Same as figure 4, but for four dimensions.

Havlin and Nossal (1984)). We find

$$d_F = d - \frac{\beta}{\nu} = \begin{cases} 2.51 \pm 0.02 & (d=3) \\ 3.05 \pm 0.05 & (d=4) \end{cases} \tag{14}$$

$$\hat{d} = z_1 d_F = \begin{cases} 1.82 \pm 0.02 & (d=3) \\ 1.88 \pm 0.03 & (d=4). \end{cases} \tag{15}$$

(Notice that equations (3) and (4) of Grassberger (1985) only hold for $d = 2$.)

In order to obtain the exponents β, ν and ν_t individually, we have fitted $\langle x_t \rangle$ to the scaling ansatz

$$\langle x_t \rangle \simeq t^{z_1} \phi(\varepsilon t^{1/\nu_t}) \tag{16}$$

following from equation (10) (these fits also helped in estimating the errors in equations

(3)-(9)). We obtained

$$\left.\begin{aligned}\nu_t &= 1.22 \pm 0.06\\ \nu &= 0.88 \pm 0.05\\ \beta &= 0.43 \pm 0.04\end{aligned}\right\} \qquad (d=3) \tag{17}$$

$$\left.\begin{aligned}\nu_t &= 1.10 \pm 0.04\\ \nu &= 0.68 \pm 0.03\\ \beta &= 0.65 \pm 0.04\end{aligned}\right\} \qquad (d=4). \tag{18}$$

When comparing the above values with previous results, we have the general problem that results of different papers are sometimes mutually exclusive.

Let us first discuss the case $d=3$. The best agreement is for the exponent ν whose world average is (Heermann and Stauffer 1981, Gaunt and Sykes 1983, Saleur and Derrida 1985) $\nu = 0.89 \pm 0.01$. (Here, our error bar is bigger mainly because we made runs only very close to p_c.) Accepting this value, some of our other error bars would become considerably smaller: $\nu_t = 1.23 \pm 0.02$, $\beta = 0.44 \pm 0.03$.

Agreement for the exponents β and η (for $d=3$) is much worse. This seems to be related to the uncertainty of p_c, together with the strong dependence of estimates of β on p_c. The best previous estimate of p_c is $p_c = 0.2492 \pm 0.0002$ (Wilke 1983) which is about 3 SD higher than our value, but values lower than ours can also be found in the literature (Heermann and Stauffer 1981). Our value of η is between those of Margolina *et al* (1982) and Gaunt and Sykes (1983) which both quote errors comparable to ours. A re-analysis of these papers (Adler 1984) claims that the errors in both were underestimated, so that our result would be the most precise one (provided our errors are not equally underestimated). Indeed, our results agree with those of Adler (1984). They also agree with the very recent value $\beta/\nu = 0.48 \pm 0.01$ of Sahimi (1985).

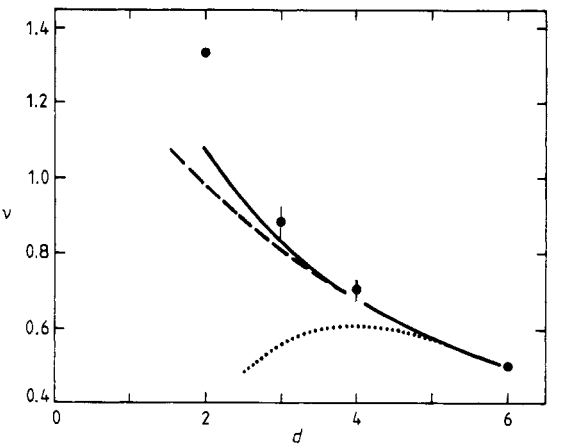

Figure 7. ε expansion for the exponent ν, compared to Monte Carlo results. Broken curve: second-order expansion (equation (19) truncated after third term); dotted curve: equation (19) truncated after fourth term; full curve: resummation of third-order expansion (de Alcantara Bonfim *et al* 1981); full circles: Monte Carlo results of present work ($d=3, 4$) and exact values ($d=2, 6$).

We should add that we found a very strong dependence of z_2 on the chosen value of p_c, much stronger than the dependence of z_1. From figure 4 we find $z_2 = 0.63 - 430(p_c - 0.248\,65) \pm 0.01$ and $\eta = -0.02 - 1300(p_c - 0.248\,65) \pm 0.03$. Similar (although less strong) dependence was found by Gaunt and Sykes (1983). It definitely eliminates values of p_c like those quoted in Wilke (1983) and Gaunt and Sykes (1983).

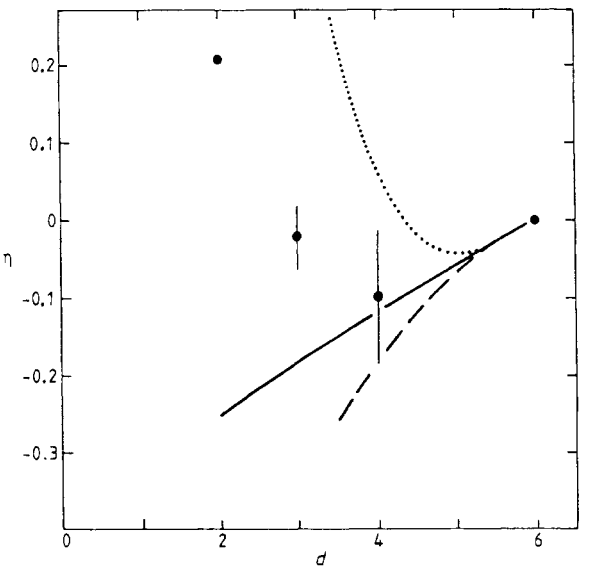

Figure 8. ε expansion for the exponent η. Meaning of curves and circles as in figure 7.

In four dimensions, the most precise previous determination of p_c is due to Adler *et al* (1984). From series extrapolations, they obtained $p_c = 0.1603 \pm 0.002$. This agrees perfectly with our value, as does the somewhat less precise value $p_c = 0.1600 \pm 0.0005$ of Stauffer (1985). For the exponent $\gamma = d\nu - 2\beta$, Adler *et al* (1984) give $\gamma = 1.44 \pm 0.05$, while Gaunt and Ruskin (1978) obtained $\gamma = 1.48 \pm 0.08$. Both agree with our result $\gamma = 1.43 \pm 0.07$, while the older MC result of Kirkpatrick (1976) is somewhat too high. The last author also found a considerably smaller value of β (0.52 ± 0.03) than we do. Finally, we should add that there is a similarly strong correlation between p_c and z_2 (and thus also between p_c and η) as in three dimensions. Accepting for example the central value $p_c = 0.1603$ of Adler *et al* (1984), we would obtain $\eta = -0.3$, a value hardly compatible with the ε expansion (see below).

Kinetic exponents for $d = 3$ and $d = 4$ have only been obtained previously by Alexandrowicz (1980). Statistics were much lower there, and p_c was only known very roughly. It thus seems unclear why quoted errors in that paper are in most cases comparable to ours (one reason is that we have taken into account corrections to scaling, while Alexandrowicz has not). Agreement is fair in most cases.

Finally, let us compare our results with ε expansions. With $\varepsilon = 6 - d$, these read (Amit 1976, Priest and Lubensky 1976, de Alcantara Bonfim *et al* 1981)

$$\nu = \tfrac{1}{2} + (5\varepsilon/84) + 0.151\varepsilon^2 - 0.009\,56\varepsilon^3 + O(\varepsilon^4) \tag{19}$$

$$\eta = -(\varepsilon/21) - 0.0222\varepsilon^2 + 0.0313\varepsilon^3 + O(\varepsilon^4) \tag{20}$$

and (Grassberger and Cardy 1985, Janssen 1985)

$$z_1 = \tfrac{1}{2} + (\varepsilon/24) + 0.0125\varepsilon^2 + O(\varepsilon^3). \tag{21}$$

These expansions and resummations thereof (de Alcantara Bonfim *et al* 1981) are compared with our Monte Carlo results in figures 7–9. We see that the exponents ν and z_1 do not present any problem. The situation for η is different, since the ε expansion converges slowly there. In view of this, our values of η seem fully acceptable, in contrast to the value of Kirkpatrick (1976) (see Amit 1976, de Alcantara Bonfim *et al* 1981).

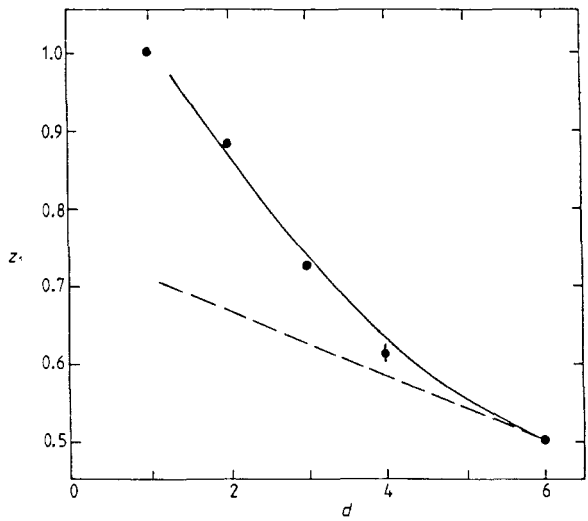

Figure 9. ε expansion for the exponent z_1, compared to Monte Carlo results. Broken line: first-order expansion (first two terms of equation (21)); full curve: second-order expansion (first three terms); full circles: Monte Carlo results of present work ($d = 3, 4$), exact values ($d = 1, 6$), and result from Grassberger (1985) ($d = 2$).

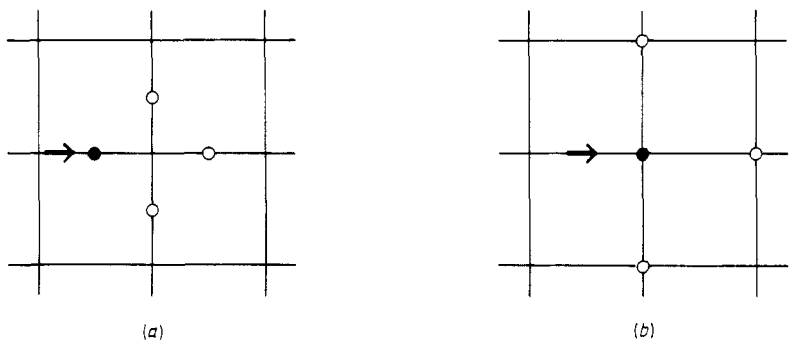

Figure 10. Basic building blocks of (*a*) bond and (*b*) site percolation, when considered as a growth process as in the present paper. In both cases, we consider as a 'basic building block' the set of all potential blocking units (open circles) reached from one penetrable unit (full circles). The arrows indicate the direction of spreading.

In addition to the above simulations of bond percolation, we have also made a few test runs with site percolation. They were very much faster, but they also showed larger fluctuations. The reason for this seems to be that the basic length scale for site percolation is twice that for bond percolation, as indicated in figure 10. In consequence, we also expect finite-size corrections to be more important for the site case. Since our basic limitations were in storage space rather than in CPU time, we did not pursue site percolation.

In conclusion, the present paper has presented results of a novel Monte Carlo method for studying percolation in three and four dimensions. The results were at least competitive with previous results, although we used a modest amount of computer time (~35 h on a CYBER 170/720, and 5 h on a CYBER 7600).

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