Monte Carlo Estimates of Percolation Probabilities for Various Lattices

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We present in this paper Monte Carlo estimates of the percolation probability $P(p)$ as a function of the constant probability p of transmitting fluid for the atom (site) and bond percolation problem for a number of lattices.

PERCOLATION deals with the flow of fluid through a medium when the flow is governed by a random mechanism residing in the medium. A medium is defined as an infinite set of *atoms* (nodes) and *bonds* (arcs) such that every bond connects two atoms. Bonds may be one-way or two-way and fluid cannot flow against the direction of a one-way bond. Fluid flowing along a bond will "wet" its two end points.

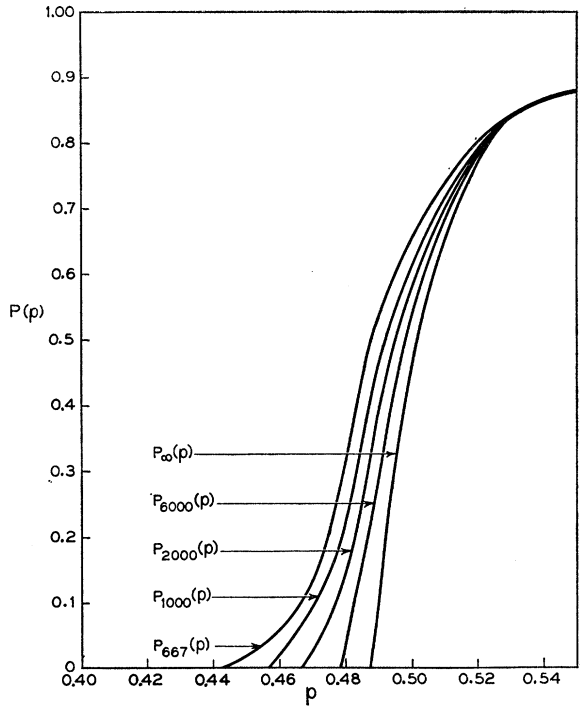

FIG. 1. Comparison of $P_N{}^B(p)$ for the two-dimensional square lattice for various values of N.

Two important distinct types of percolation are (a) atom percolation and (b) bond percolation. In (a) each atom A has a constant probability p of allowing fluid reaching A to flow along bonds *from* A. In (b) each bond has a constant probability p of transmitting fluid. For the various physical applications of these processes see Domb,[1] Elliott *et al.*,[2] Sato *et al.*,[3] and Broadbent and Hammersley.[4]

The *percolation probability* $P(p)$ of the medium is defined to be the probability that fluid supplied to a single specified atom in the interior of the medium will "wet" infinitely many others. The *critical probability* p_0 is defined as

$$p_0 = \sup_{P(p)=0} p. \tag{1}$$

Wherever necessary we use $P^A(p)$, $p_0{}^A$, $P^B(p)$, $p_0{}^B$ to distinguish between atom and bond processes.

This paper presents and discusses results obtained

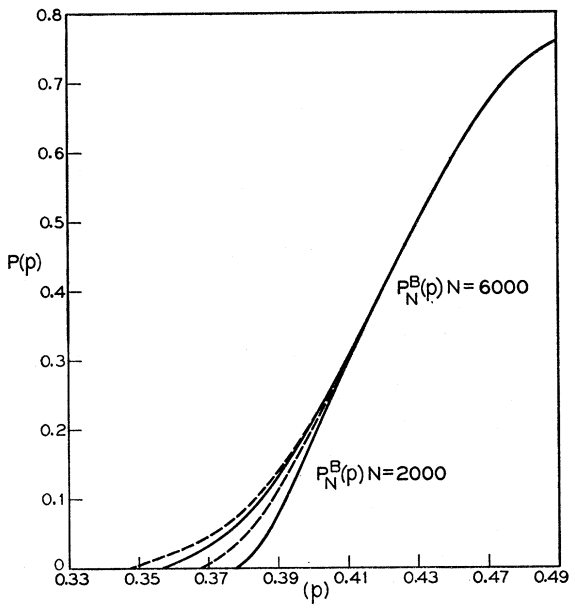

FIG. 2. Comparison of $P_N{}^B(p)$ for a typical three-dimensional lattice for various values of N.

[1] C. Domb, Nature **184**, 509 (1959).
[2] R. J. Elliott, B. R. Heap, D. J. Morgan, and G. S. Rushbrooke, Phys. Rev. Letters **5**, 366 (1960).
[3] H. Sato, A. Arrott, and R. Kikuchi, J. Phys. Chem. Solids **10**, 19 (1959).
[4] S. R. Broadbent, J. M. Hammersley, Proc. Cambridge Phil. Soc. **53**, 629 (1957).

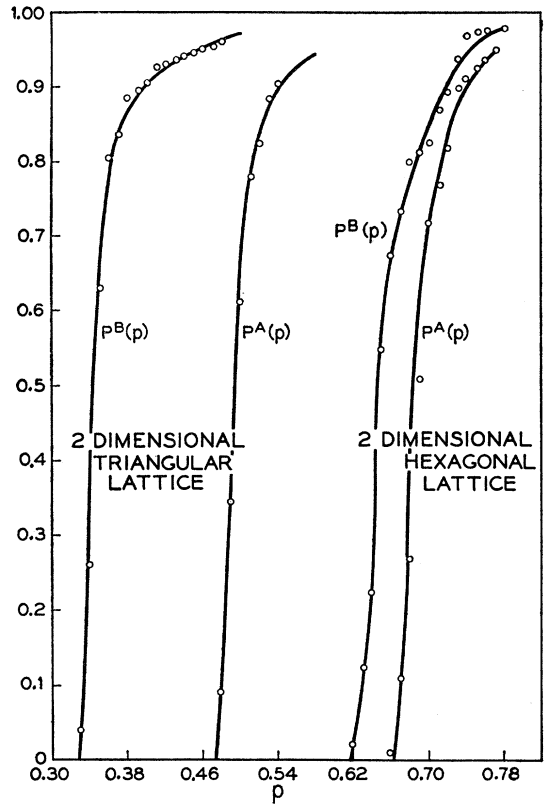

FIG. 3. Comparison of $P^B(p)$, $P^A(p)$ for the two-dimensional triangular and hexagonal lattices.

for $P(p)$ by a Monte Carlo experiment on the IBM 7090 computer at Bell Telephone Laboratories. The corresponding results obtained for p_0 have already been published.[5,6] The method of computation depends upon the fact that, if $P_N(p)$ denotes the probability of a single source wetting at least N atoms, then for sufficiently large N, $P_N(p)$ approximates $P(p)$. For complete details, see Frisch *et al.*[7]

The size of the computer's store sets an upper limit on the practicable value of N; and, within this limit, the larger N, the longer the computing time is. Hence, N should be chosen as small as possible consistent with yielding an adequate approximation to $P(p)$ by $P_N(p)$. A previous calculation at Harwell for the three-dimensional simple cubic lattice, on a machine whose store would accept a maximum $N=8192$, had indicated that values of N about 2000 would suffice.[8] The IBM 7090 calculations at Murray Hill, where the store accepted a maximum $N=7000$, supported this finding for the three-dimensional lattices examined. However, it also indicated that larger values of N were needed for two-dimensional lattices. We have not yet evinced any theoretical explanation of this empirical fact. Figure 1 shows curves for $P_N{}^B(p)$ for various values of N on the two-dimensional square lattice, and it also shows an estimate of $P^B(p)$ obtained from these curves by extrapolation in $1/N$. This estimated $P^B(p)$ is positive for $p\geq 0.487$, but it is known[9] theoretically that $P^B(p)=0$ for $p\leq\frac{1}{2}$. Some of this contradiction may be ascribed to Monte Carlo sampling errors, but we do not think that the whole of the discrepancy can be explained away like this. A similar discrepancy appears for the two-dimensional triangular and hexagonal lattices, where the Monte Carlo curves conflict with the theoretical result[10] that the two respective bond problem critical probabilities must sum to at least 1. In comparison with Fig. 1, Fig. 2 shows the much more rapid convergence of $P_N(p)$ to $P(p)$ in a typical three-dimensional case.

The Monte Carlo results satisfy $P^A(p)\leq P^B(p)$ for each lattice in conformity with theory.[11] The strongest and weakest cases of this inequality are illustrated in Fig. 3 and these support the belief that, for these eight lattices, $P^A(p)$ is strictly less than $P^B(p)$, $(p_0<p<1)$.

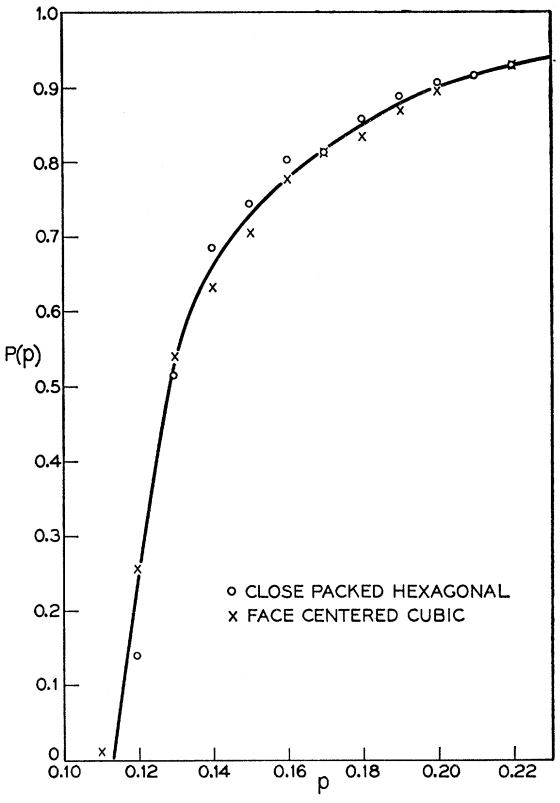

FIG. 4. Comparison of $P^B(p)$ for the face-centered cubic and close-packed hexagonal crystals.

[5] V. A. Vyssotsky, S. B. Gordon, H. L. Frisch, and J. M. Hammersley, Phys. Rev. **123**, 1566 (1961).
[6] H. L. Frisch, E. Sonnenblick, V. A. Vyssotsky, and J. M. Hammersley, Phys. Rev. **124**, 1021 (1961).
[7] H. L. Frisch, S. B. Gordon, J. M. Hammersley, and V. A. Vyssotsky, Bell System Tech. J. **42**, May (1962).
[8] J. M. Hammersley, *Methods in Computational Physics* (to be published).
[9] T. E. Harris, Proc. Cambridge Phil. Soc. **56**, 13 (1960).
[10] M. E. Fisher, J. Math. Phys. **2**, 620 (1961).
[11] J. M. Hammersley, J. Math. Phys. **2**, 728 (1961).

The curves for the face-centered cubic and close-packed hexagonal lattices in Fig. 4 are indistinguishable to within Monte Carlo sampling errors. We conjecture that these two curves should be theoretically identical and that a similar identity should hold for the $P(p)$ of the two tetrahedral lattices (ice and diamond).[11a]

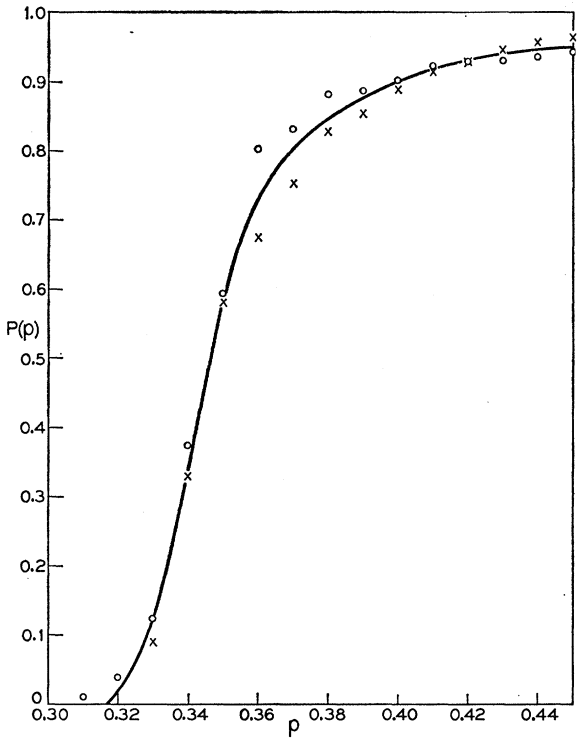

FIG. 5. Comparison of $P^B(p)$ for the triangular lattice derived from two completely different samples.

Each curve is effectively a histogram for a population of 100 independent observations (save that 50 replaces 100 in the case of $P^A(p)$ for the ice-tetrahedral, the face-centered cubic, and the close-packed hexagonal lattices). The standard error of P associated with a single point on any curve is thus $[P(1-P)/100]$ or $[P(1-P)/50]$ as the case may be. Figure 5 exhibits two independent experiments for the triangular lattice, shows that the discrepancy between these experiments conforms to this standard error, and illustrates the relative accuracy to be expected in the estimates here and in the other figures.

[11a] *Note added in proof.* There is evidence that this conjecture is false due to M. E. Fisher (private communication).

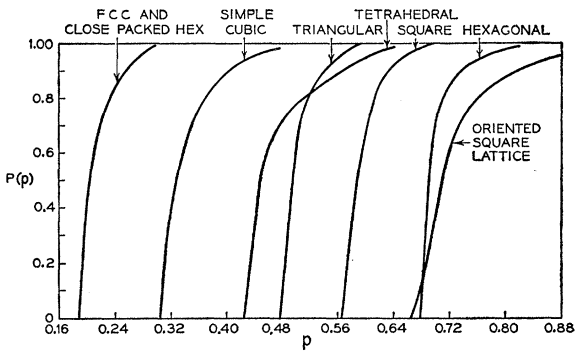

FIG. 6. $P^A(p)$ for the nine structures.

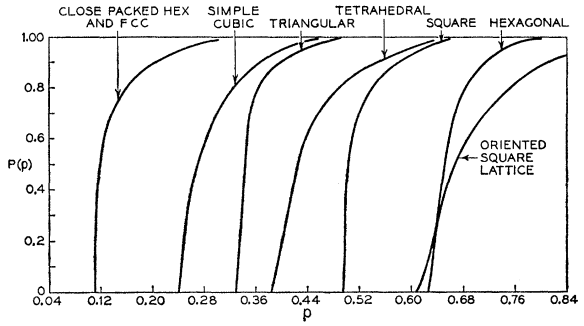

FIG. 7. $P^B(p)$ for the nine structures.

Figures 6 and 7 provide a summary of results. All lattices have two-way bonds, with the exception of the oriented square lattice. In this exceptional case, each atom has plane coordinates $(x, y=0, 1, 2, \cdots)$ and a pair of bonds from (x,y) to $(x, y+1)$ and to $(x+1, y)$. The critical bond probability for this oriented lattice agrees with Mauldon's theoretical result.[12]

Complete numerical results for $P(p)$ may be obtained on request from Bell Telephone Laboratories.

[12] J. G. Mauldon, *Proceedings of the Fourth Berkeley Symposium on Mathematical Statistics and Probability* (to be published).