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Percolation of Chains and Jamming Coverage in Two Dimensions by Computer Simulation

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A computer simulation model is used to study the percolation of random chains with a self-avoiding constraint. The percolation threshold is found to decay with the chain length L_c with a power law $L_c^{-0.1}$, while the jamming coverage varies as $L_c^{-1/3}$.

KEY WORDS: Percolation; chains; jamming coverage.

Inhomogeneous fractals are relevant to understanding many processes involving spatial growth and temporal evolution from small-scale (i.e., materials growth) to large-scale geological and astronomical phenomena such as secondary methods of oil recovery, crack propagation, galactic cluster formation, etc.[1-5] In particular, percolation has been an area of acrtive research because of its applications to the problems of fluid flow through porous media[1] and sedimentation. Site and bond percolation have been extensively studied, and have been successful in improving our understanding of the permeability of sediments.[1] In some sediments, such as sandstone, the basic structure is composed of single grains of sand which are modeled quite well using site and bond percolation. Other sediments, such as clay, have a flat, platelike structure which is not well suited to modeling via site and bond percolation because the mechanisms of site and bond percolation cannot describe the different conformations which clay

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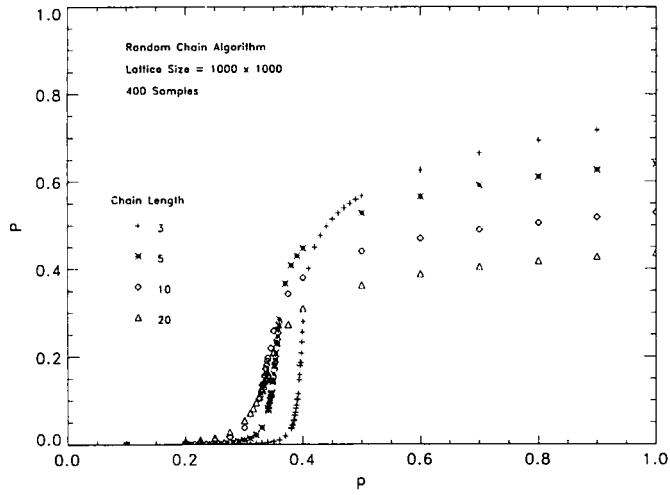
particles are known to acquire. These conformations are known to be correlated to the sedimentation processes which lead to a percolating porous medium. Consideration of random chains as the percolating units would be a natural extension of site, bond, and rod[6] techniques in order to study the effect of conformation on the percolation.

Drory *et al.*[7] studied the percolation threshold of permeable objects of various shapes in continuum space. They found that the percolation threshold depends strongly on the sizes and shapes. In a previous paper[6] we investigated the percolation of stiff chains (sticks or thin rods) of various sizes in a two-dimensional discrete lattice and found a strong dependence of the percolation threshold on the chain length. Here we extend this study to random chain percolation and jamming coverage in two-dimensional lattices.

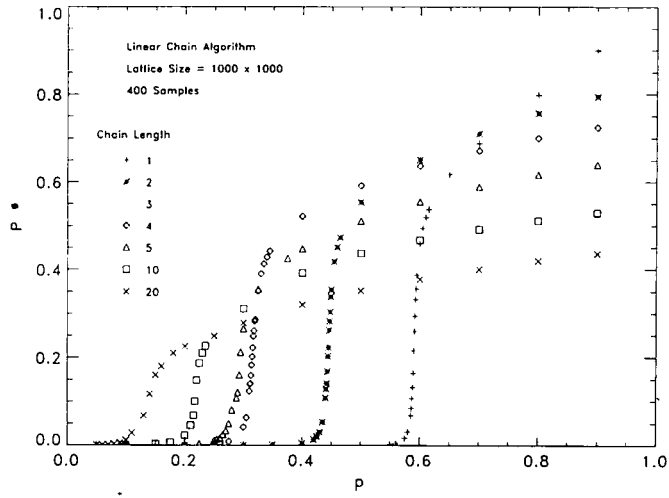
We consider a square lattice and constrained random chains with self-avoiding-walk-like (SAW) conformations aas the percolating units. In contrast to a rigid rod of fixed length L_c as a percolating unit where L_c sites are connected in a linear fashion, we consider a random chain generated on the trail of a random walk of L_c steps with a self-avoiding constraint as a percolating unit. Thus, the length of a chain L_c is the number of connected sites on the lattice; $L_c = 1$ corresponds to the standard site percolation. For a fixed chain length L_c, we generate clusters of connected chains in the following way. We select an empty site and the decision to place a chain beginning at this site is determined with a probability p using a pseudo-random number generator. If the random number is less than or equal to p, then we attempt to generate a constrained SAW-like chain of length L_c. The chain is then placed if no occupied lattice site is in the way (i.e., two chains are not allowed to share a lattice site). If our attempt to place a random chain fails, then we move to the next empty site and repeat the above process. This process of selecting an empty site with probability p and an attempt to place is repeated for all lattice sites. The consequence of this rule is that a jamming concentration limit p_j is reached when it is not possible to place additional chains in the lattice.

A cluster is formed by joining the nearest neighbor occupied sites. Thus, two neighboring chains will be part of the same cluster if they are separated by one lattice constant. We concentrate on the percolation quantities such as the cluster size distribution, percolation probability, and the second moment of the cluster size distribution. The jamming coverage is the maximum percolation probability for the chain length L_c, where L_c is larger than one.

Initially the simulations were carried out on a CRAY YMP8 machine. The lack of floating point computations and the small amount of vector code in the algorithm proved to be an inefficient program on the CRAY.



A.



B.

Fig. 1. Percolation probability versus concentration; (A) random chain and (B) rod (with chain lengths of 10 and 20 corrected from ref. 6).

A more efficient solution was to distribute the applications across eight Silicon Graphics Indigo workstations using the PVM software package.[8] The parallelization was done at the coarsest level of granularity in that each workstation independently performed calculations for 50 realizations and then the results were collected and averaged to produce the final average. In a typical computation we used 400 independent realizations for monodispersed chains of a fixed length for each concentration in order to evaluate the percolation quantities. The CRAY required approximately 30 min of a single CPU to perform the computation on a 1000×1000 lattice at a single concentration. The Silicon Graphics/PVM solution required about 1 hr elapsed time with each workstation contributing about 45 min of CPU time to perform the 50 realizations. Clearly this is not typical of all programs, only programs without floating point calculations or vector code and having coarse granularity should expect this type of performance.

A typical plot of the percolation probability P versus concentration p is shown in Fig. 1A; for comparison we present a similar plot for the rod/stick percolation.[6] Note that the dispersity in the variation of the percolation threshold with the chain length is slightly smaller in chain percolation (Fig. 1A) than in the rod percolation (Fig. 1B); this is due to the fact that the percolation threshold for the chain percolation is lower than that for the rod percolation of the same length. We have also studied the second moment of the cluster size distribution, i.e., the "susceptibility," an analog of magnetic systems, to estimate p_c. However, the variation of the

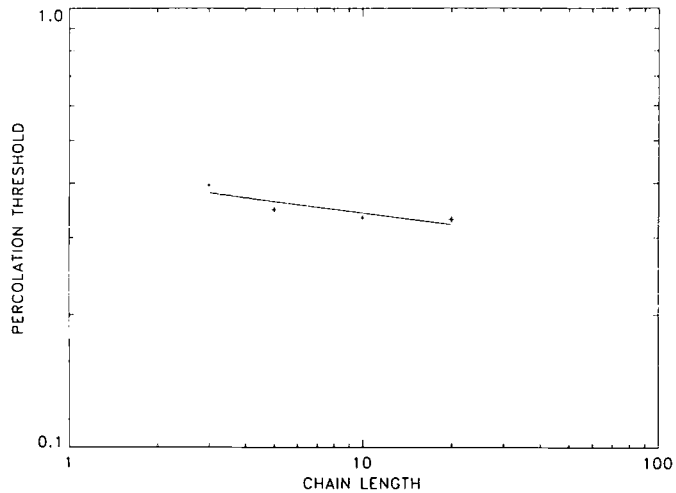


Fig. 2. Percolation threshold versus chain length L_c.

percolation threshold p_c with the chain length L_c shows a power-law decay $p_c \sim L_c^{-0.1}$ as shown in Fig. 2, which differs from the power law found for rod percolation, where $p_c \sim L_c^{-1/2}$.[6]

As we have mentioned above, we define the jamming coverage p_j as the saturated percolation probability where the chains are jammed. The saturated coverage decreases on increasing the chain length. Figure 3 shows such a power-law decay of the jamming coverage with the chain length, i.e., $P_j \sim L_c^{-1/3}$ (the slope is -0.278). This agrees with the power law found for the jamming coverage in rod percolation ($P_j \sim L_c^{-1/3}$; slope is -0.277). Numerous studies have been carried out in recent years on the random sequential adsorption where the power-law approach to the asymptotic value of the satured coverage in the long-time ($t \to \infty$) regime and its dependence on the aspect ratios and shape of the deposited species have emphasized.[9-16] In the random sequential absorption of unoriented rectangles of an aspect ratio of α, Vigil and Ziff have found that the jamming coverage has a maximum at $\alpha = 2$ and varies as $\alpha^{-0.22}$ as $\alpha \to \infty$.[11] We point out that the percolation of chains in our model is different from that of Bradley *et al.*[17]

It is tempting to mention that our simulation may have some application in understanding the variation of the critical density of alkanes with the carbon number.[18,19] The alkanes are short-chain molecules, and the chain (of length L_c) of our simulation may be a good approximation for modeling the conformation of normal alkanes with carbon units of the

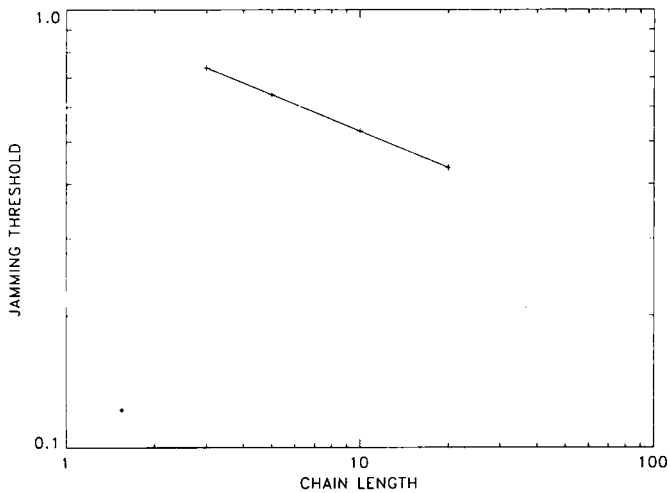


Fig. 3. Jamming coverage versus chain length L_c.

Table I. Percolation Exponents for Various Chain Lengths[a]

L_c	p_c	β	γ	ν	D
3	0.40	0.20	1.3	0.83	1.8
3 (rod)	0.37	0.14	1.9	1.3	1.9
5	0.35	0.22	1.3	0.88	1.8
5 (rod)	0.29	0.14	2.0	1.3	1.9
10	0.33	0.16	1.7	0.99	1.8
10 (rod)	0.24	0.14	2.2	1.3	1.9
20	0.33	0.14	1.6	0.93	1.9
20 (rod)	0.13	0.14	2.4	1.3	1.9

[a] Included for comparison are the percolation exponents from percolating rods for various chain lengths from ref. 6.

order of 5–20. Our simulation is done on a square lattice without considering the realistic interactions and energetics of the thermodynamics; therefore, it is not possible to compare these results qualitatively with both experimental data[19] or thermal Monte Carlo data.[18] However, the decay of the critical concentration and the jamming coverage with the chain length has qualitative similarity with the decay of critical density of the normal alkanes with the carbon number (see Fig. 4 of ref. 18). Thus the conformation and the length of alkanes[20] may be important in understanding their packing and phase equilibria.

We have estimated the exponents β, γ, and ν for the percolation probability, second moment of the cluster size distribution, and the correlation length, respectively, for the percolation phase transition for various chain lengths; these values are presented in Table I. We have used $D = d - \beta/\nu$ to evaluate the fractal dimension D of the percolating cluster at the percolation threshold ($d = 2$). The variation in the value of the exponents with the chain length suggests that there are considerable fluctuations in these estimates. Within the limits of the fluctuations we find that these exponents are not different from their corresponding estimates for the rod percolation.

In summary, we have studied the percolation of the constrained SAW-like chains in a random sequential adsorption. The percolation threshold decays with the chain length as $L_c^{-0.01}$ and the jamming coverage as $L_c^{-1/3}$. The type of chain (rod or flexible) does seem to affect the power laws for the percolation threshold, while it does not affect the power laws for the jamming coverage.

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