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Difference percolation on a square lattice

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Abstract

Simulations of percolation processes on random site square lattices are performed implementing a different occupation algorithm for both ordinary percolation (OP) and invasion percolation (IP) problems. The main feature of the occupation process is the fact that it is performed in a locally restricted way by inspecting the difference between the measure assigned to neighboring sites. This restriction carries an intrinsic change in the distribution of invaded sites with a different percolation threshold and the same universality class. Conclusions are drawn concerning physical problems of propagation phenomena with local barriers where these simulations prove the possibility of controlling the wide spread of the invasor. © 2000 Elsevier Science B.V. All rights reserved.

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1. Introduction

Many physical phenomena can be modeled through classic and invasion percolation processes. Examples of these range from viscous flow of a liquid phase into a bed of glass beads to the problem of water leakage or oil recovery in a sedimentary rock. In particular, invasion percolation phenomena have been an object of intensive study during the last two decades due to both pure statistical mechanics interests and important technological applications [1–6].

In some real problems, the presence of fields or topological features makes the description of the dynamics of the system more complicated than the one given by classical percolation and invasion percolation models. For that reason, one can find

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works in the literature that try to take into account some of these aspects by introducing modified algorithms [6–8]. One example is the multiple invasion percolation model developed by Onody et al. In that model a certain number of lattice sites can be simultaneously invaded during one invasion step. Other works deal with the problem of a classical invasion percolation process onto a correlated lattice trying to account more realistically for the dynamics of a fluid displacement through a rock reservoir, where spatial correlations are frequently present [6,9,10].

Despite that, there are still open questions in this field like, for instance, what happens if the occupation of a given site depends on locally defined rules, or, in other words, if the occupation of the site depends on its surroundings? Is there any possibility of frustration for some occupation conditions or rules?

In the present work, simulations of percolation processes on random site square lattices are performed implementing a different occupation algorithm for both ordinary percolation (OP) and invasion percolation (IP) problems.

Assume a site network with d-dimensional measure $\mathbf{r}$ assigned to each of the sites. Each vector component in each d-direction is sampled randomly from a uniform distribution in the interval $(0,1)$. One must not confound the random vector $\mathbf{r}$ with the lattice itself, i.e., with the lattice site positions. One can think of a physical process whose propagation through the network will depend on $|\mathbf{r}_i - \mathbf{r}_j|$ to be less than some given value δ. In other words, assuming that the process is already occurring at site i, it will proceed through junction ij only if $|\mathbf{r}_i - \mathbf{r}_j| < \delta$. If this condition is fulfilled, the process will also occur at site j, and so on. The results presented here correspond to the one-dimensional problem, i.e., scalar measure of lattice sites (one-component vectors $\mathbf{r}$).

We can relate this one-dimensional case with interesting physical processes where the propagation of a quantity through a system depends just on local differences between the nearest neighbors. Continuum percolation is an example, where the spanning cluster is built with those discs whose centers are close enough to touch or overlap each other [11–13]. Another example is the propagation of a disease where it is necessary to stay at a given local distance from an already infected specimen in order to become sick. Furthermore, there exist physicochemical problems like, for instance, ion exchange techniques to determine Cu surface areas where the testing molecule (N_2) cannot adsorb if the distance between two neighboring metallic atoms is greater than some critical value [14,15].

The difference algorithm will be presented in the next section. Then, results and discussion will be addressed for the cases under study. Conclusions and future perspectives will be presented in the last section.

2. Difference percolation algorithms

The main feature of these algorithms is the fact that occupation is performed in a locally restricted way. In IP standard algorithms a site belonging to the interface of occupied–unoccupied elements is occupied if it is of the lowest value, whereas, in

OP the site is occupied if its value is less than the occupation probability. Here, the necessary condition to occupy a site is tested on the difference between neighbors. In the case of OP, this difference is compared to a fixed parameter. For IP, the front will invade the least difference at the interface. In what follows, the way simulations were performed is explained and the algorithms will be clarified.

Numbers between 0 and 1 are randomly assigned to the sites of a square network. These numbers are sampled from a uniform distribution. In all the present simulations the occupation process always begins through the central site in the network (one-site cluster) and a breakthrough is achieved when the percolating front first touches one of the lattice edges. No trapping is allowed.

A local rule is imposed through a parameter δ that can take any value belonging to the interval $(0,1)$. Once δ is chosen, it remains fixed for the rest of the run. If a non-occupied site belonging to the occupied–unoccupied interface with a random number r_1 has an already occupied neighbor whose measure is r_2 in such a way that $|r_1 - r_2| < \delta$, it can be occupied, otherwise, it cannot. This will be the first condition checked before performing any occupation step in any of the algorithms presented here.

The following question then arises: which is the lowest value for δ needed for the cluster to percolate?

To study the effect of this restriction in the percolation patterns three different cases were studied.

Case A: Multiple occupation. Each already occupied site belonging to the interface is visited. Assume that it has a measure r. All its unoccupied nearest neighbors are inspected: if a neighbor has a value that belongs to the interval $r \pm \delta$, it is automatically occupied. Thus, multiple occupation can occur. Once all the neighbors are checked, the site is killed. Then, another site is visited until all the sites of the interface are inspected. To kill a site means that after all its neighbors have been inspected for the δ-condition to be fullfilled, it is no more useful to consider that site as a part of the active interface. A set of 500 equivalent runs was performed for each δ value and square site networks of (1000×1000) size were used.

Case B: Occupation of the minimum neighbor. Each already occupied site on the network is visited. All its neighbors are inspected as explained above; however, in this case, only the neighbor with the minimum measure out of the ones fulfilling the δ-condition, is occupied. Thus, at the most one neighbor per site is occupied in each step. After the inspection of the neighbors, the site is no longer useful and then killed as in case A. Consequently, the occupation propagates through a one-dimensional path according to the minimum measure route within the δ-condition. If the site being visited does not have at least one neighbor fulfilling the required condition, then the process stops because there is no way to continue it and the entire sample is discarded.

Simulations on (1000×1000) site networks were performed using uniform distributions of random numbers. The results were averaged over 500 equivalent runs for each δ value used.

Case C: Invasion percolation. In this case, the invasion is performed with a classical invasion percolation algorithm. Accordingly, no multiple invasion occurs and no sites

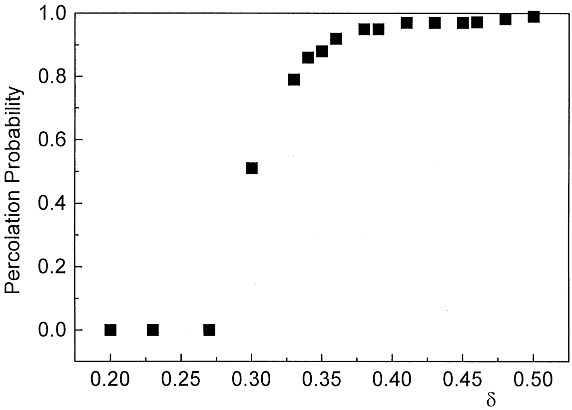

Fig. 1. Percolation probability as a function of δ. Breakthrough is not achieved until δ is greater than a critical value of the order of 0.27.

are deleted. Here, the invasion front advances through the site at the interface with the smallest difference $\delta_{\mathrm{ij}} = \min|r_i - r_j|$ between its random measure, r_i, and the one r_j of its already invaded neighbor. This means that there is no externally imposed δ value, the system by itself will look for the smallest one at the interface.

Simulations were run over (500×500) site networks and results were averaged over 10^3 samples.

The quantities measured for the three cases were the percolation probability, the dependence of the spanning cluster's mass on the gyration radius, and the density of the invaded sites as a function of their measure. The results obtained as a function of δ and for each case are presented and discussed in the next section. Statistical uncertainty is less than 0.4% in all the results shown below.

3. Results and discussion

Case A. Simulations for δ values ranging from 0.2 to 0.5 were done. The percolation probability as a function of δ is plotted in Fig. 1. As can be seen, breakthrough is not achieved until δ is greater than a critical value. We can define a critical threshold, δ_{c}, as the value of δ for which the percolation probability is for the first time different from zero (recall the initial finite cluster seed) thus, from Fig. 1, $\delta_{\mathrm{c}} = 0.27$. This behavior shows two important aspects. First, it seems that the system can easily percolate when multiple invasion is performed into all the neighbors related "locally" with an already invaded site through the δ-condition with $\delta > \delta_{\mathrm{c}}$. Finite-size effects must be taken into account in order to establish with a good accuracy the value for δ_{c}. In the present simulations finite-size trends are hard to detect for network sizes > 1000.

Secondly, to know the δ values which make the invasion cluster unable to percolate is an important aspect to take into account when a physical problem of propagation

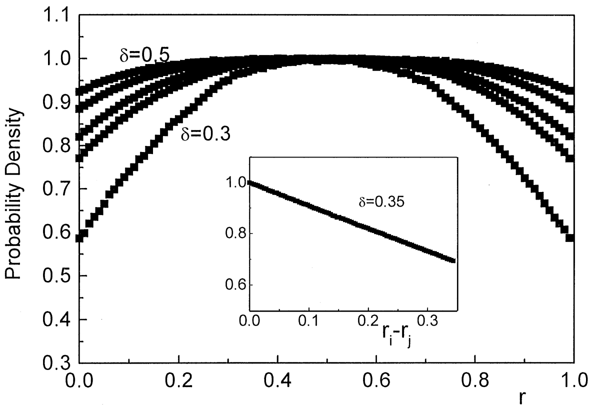

Fig. 2. Probability density profile of occupied sites as a function of their random values for $\delta = 0.3, 0.37, 0.4, 0.45$ and 0.5. These values are indicated explicitly only for the extreme cases 0.3 and 0.5. Each frequency profile is normalized by its most probable value. The inset shows the same profile as a function of the difference between the values of the sites.

phenomena with local barriers is modeled because these simulations prove the possibility of frustration of the information propagation, or, in other words, the possibility of controlling the wide spread of the invasor. This range is not very much affected by finite-size effects in the sense that, at most, the critical threshold will move to greater values of δ.

A study of the behavior of the cluster's mass dependence on the gyration radius was performed for different values of δ. As known, the mass M (number of invaded sites) scales as $M \sim R^{d_f}$, where d_f is the fractal dimension of the cluster. Only for $\delta = 0.3$ the cluster presented a fractal structure with $d_f = 1.91$, but, for greater values of δ, it was completely compact with $d_f \sim 1.99$ for all δ values.

A more interesting behavior was found for the probability density of occupied sites as a function of their measure. Fig. 2 shows this behavior for several values of δ. There, each frequency profile is normalized by its most probable value. For classic IP in a finite network, for instance, this probability density profile is close to a step function where the discontinuity is located at the critical ordinary percolation threshold $p_c = 0.5928$ [8,16]. But here it is not expected to occur that way because of the difference in the occupation rules, and, in fact, we can see that the profile can easily be fitted by a parabolic function centered at $r = 0.5$ and their widths increase with δ. Thus, one is able to span a cluster with an acceptance profile that can be described by a particular parabolic function depending on the δ value associated with the simulated problem.

A plot of the same profile but as a function of the difference between the value of the newly occupied site and the value of the already occupied neighbor giving rise to that new occupation is shown in the inset of Fig. 2.

Case B. For all the simulations performed, occupation never reached the breakthrough stage, even for $\delta = 1$. Although the mass of the incipient cluster increases with

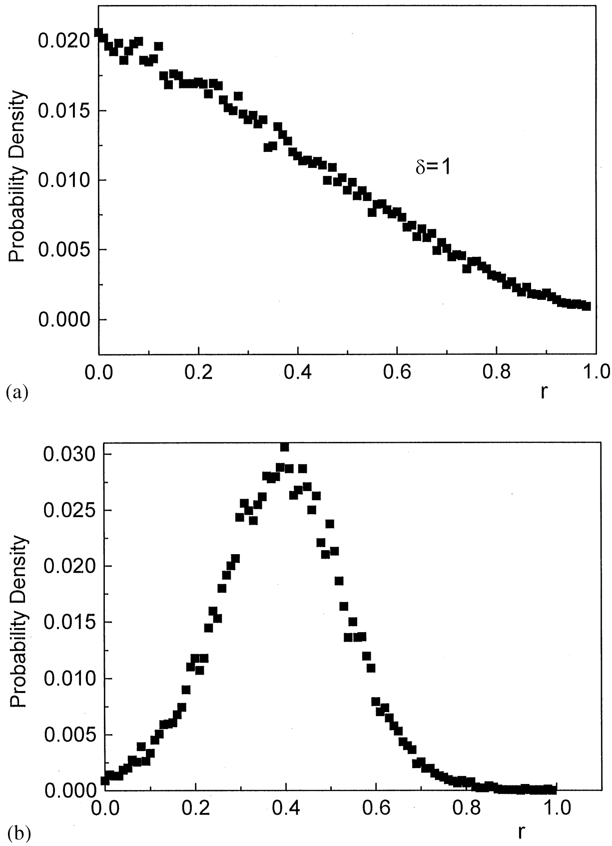

Fig. 3. Probability density profile of occupied sites as a function of their random values for case B. (a) For uniformly distributed random numbers and $\delta = 1$; (b) for Gaussian distributions and $\delta = 1$.

δ, the system does not percolate. This result demonstrates that this occupation procedure, similar to a self-avoiding random walk but through the minimum neighbor of the growing tip, is also frustrated as its random counterpart. Other random distributions of the site measure lead to the absence of percolation as well.

The main difference between the two distributions used to generate the random numbers was the occupied sites profiles. Fig. 3(a) and (b) shows the difference. For the case of uniformly distributed random numbers the profiles could be fitted by a straight line. As expected, for greater δ values the dispersion of the data was lower. Fig. 3(a) shows the profile for $\delta = 1$. On the other hand, for Gaussian distributions the profile was Gaussian. This difference in the profiles is helpful to characterize each process, i.e., if one just knows the occupied sites profiles, the complete distribution of site values can be inferred.

Case C. The invaded sites profile as a function of δ is shown in Fig. 4. As can be seen those sites with differences greater than $\delta \sim 0.3$ are never invaded and the

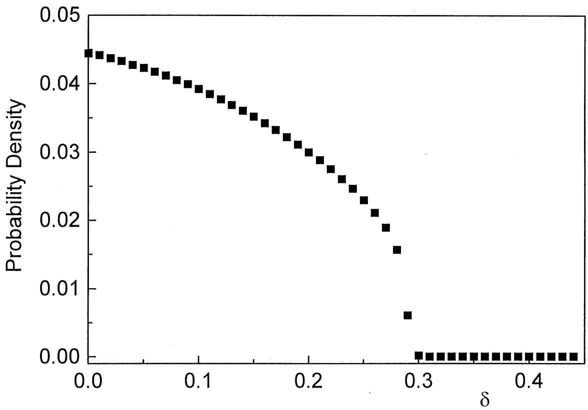

Fig. 4. Probability density profile of invaded sites for case C. Frequency is normalized.

threshold for percolation agrees very well with the one found for the OP counterpart of this model, i.e., $\delta_c = 0.27$. The shape of the curve is different from the step behavior expected in classic IP.

In what follows the mass behavior of the percolating cluster is concerned, it was found to be fractal for all $\delta \geqslant \delta_c$, and the fractal dimension found using $M \sim R^{d_f}$ was $d_f = 1.90$ for all $\delta \geqslant \delta_c$. This fractal dimension was checked more carefully by using the well-known scaling law $M \sim L^{d_f}$, where L is the size of the network. Simulations with $L = 100$–600 were performed giving a value of $d_f = 1.89$, coincident with that of invasion percolation without trapping [3]. Thus, the fractal properties of the clusters generated by this model in case C are similar to the ones of classic invasion percolation.

4. Conclusions

Simulations of OP and IP on random site square lattices were performed implementing a different occupation process. The main feature of the occupation process is the fact that it is performed in a locally restricted way by inspecting the difference between the measure assigned to neighboring sites.

The same critical values for δ were found for cases A and C. This is an important aspect to be taken into account when a physical problem of propagation phenomena with local barriers is modeled because these simulations prove the possibility of controlling the wide spread of the invasor.

With the rules defined for case A, one can sample a different profile for the invaded sites than in the conventional way, i.e., parabolic distributions.

For case B, frustrations were always found, even for $\delta = 1$.

For case C, the shape of the invaded sites profile is different from the step behavior expected in classic IP and the fractal properties of the clusters are similar to the ones of classic IP.

In conclusion, the restriction imposed by the δ-condition carries an intrinsic change in the distribution of invaded sites with a different percolation threshold although belonging to the same universality class.

At present, application of this model to characterize different π-Si surface structures is being developed with promising results [17].

These results encourage further study to introduce restricted occupation algorithms on correlated networks, to investigate the dependence of δ_c on the degree of site correlation, as well as to avoid frustrations.

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References

[1] R. Lenormand, S.Bories, C.R. Acad, Sci. Paris B 291 (1980) 279.
[2] D. Wilkinson, J.F. Willemsen, J. Phys. A 16 (1982) 3365.
[3] L. Furuberg, J. Feder, A. Aharony, T. Jøssang, Phys. Rev. Lett. 61 (1988) 2117.
[4] R.N. Onody, Int. J. Mod. Phys. C 6 (1995) 77.
[5] R.N. Onody, A.N.D. Posadas, S. Crestana, J. Appl. Phys. 78 (1995) 2970.
[6] A.M. Vidales, E. Miranda, G. Zgrablich, Europhys. Lett. 36 (1996) 259.
[7] R.N. Onody, R.A. Zara, Physica A 231 (1996) 375.
[8] R.A. Zara, R.N. Onody, Int. J. Mod. Phys. C 10 (1999) 227.
[9] A.M. Vidales, E. Miranda, G. Zgrablich, Int. J. Mod. Phys. 9 (1998) 827.
[10] M. Sahimi, M. Hashemi, J. Ghassemzadeh, Physica A 260 (1998) 231.
[11] G.E. Pike, C.H. Seager, Phys. Rev. B 10 (1974) 1421.
[12] E.T. Gawlinski, H.E. Stanley, J. Phys. A 14 (1981) L291.
[13] W.T. Elam, A.R. Kerstein, J.J. Rehr, Phys. Rev. Lett. 52 (1984) 1516.
[14] M.A. Kohler, J.C. Lee, D.L. Trimm, N.W. Cant, M.S. Wainwright, Appl. Catal. 31 (1987) 309.
[15] E.D. Guerreiro, O.F. Gorriz, J.B. Rivarola, L.A. Arrúa, Appl. Catal. A 165 (1997) 259.
[16] D. Stauffer, A. Aharony, in: Introduction to Percolation Theory, Taylor and Francis, London, 1992.
[17] A. Ferreira da Silva, R.R. Rosa, A.M. Vidales, R.H. Lopez, in preparation.