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Competing two-species directed percolation

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Abstract. We study an extension of conventional directed percolation (DP) with two species (A and B) using mean-field and Monte Carlo methods. The densities of the two species in the steady-state exhibit phase transitions which are due both to simple percolation and to competition between the species. In $1 + 1$ dimensions, as well as a simple DP transition, there is a line of first-order transitions between pure-A and pure-B phases. The phase diagram in $2 + 1$ dimensions agrees qualitatively with that obtained from mean-field calculations, with second-order transitions between pure and mixed phases. Preliminary studies suggest that the critical exponents are in the same universality class as (one-species) DP.

1. Introduction

The simplest examples of non-equilibrium systems whose steady-states display a phase transition are lattice models where a binary variable $\sigma_i = 0, 1$ is associated with each site and where the dynamical local rules for the evolution of the site variable allow for the existence of an absorbing state.

Applications range from processes of adsorption–desorption of particles on a surface (in which case $\sigma_i = 0, (1)$ can represent a vacant (occupied) site) to simplified models for propagation of epidemics or spreading of a liquid through porous medium.

In fact all the models built with a certain diversification of the local rules (A model [1], contact process [2], and cellular automata versions of them [3]) have so far been found to display the same type of critical behaviour, all belonging to the universality class of directed percolation. Field theoretical arguments exist that it should indeed be so. These arguments are also able to predict that the phase transition into the absorbing state should still have the same critical properties if the number of site variables increases [4].

However, one can envisage situations of interest where, for example, the number of site variables is three, and where different types of phase transitions take place. In such a situation, a very rich phase structure can occur, with several different order parameters exhibiting phase transitions at different points. In the framework of equilibrium statistical mechanics, such a situation is present in Blume *et al* [5] for example.

The particular case of interest in this article is a model of adsorption–desorption of two different types of particles A and B, or the spreading of two immiscible liquids

(with colours A and B) through a porous medium. The spreading of the two species is affected not only by the distribution of pores available to them, but also by the competition between species for a given pore. One then expects that the densities of the two species in the steady state will not only exhibit phase transitions which are due to simple conventional DP of either species, but also transitions due to competition between the species. The interplay between the two species is very delicate, since either or both may become critical at any given point, and might be expected to lead to phase transitions of a different type from DP, in contrast to the one-species case.

The article is organized as follows. In section 2 we define precisely the model sketched above. In section 3 we study the model in a mean-field approximation for arbitrary coordination number. As we shall see, the intermediate phases anticipated above are indeed present, at least for systems of sufficiently high dimensionality. In section 4 we obtain the phase diagram from numerical simulations. Both the one- and two-dimensional cases are studied. In section 5, the critical behaviour at one transition point is studied using Grassberger's dynamical method. It is found that the critical exponents of this model are compatible with those of DP. Finally, other interesting aspects or possible extensions of the model are discussed in the conclusion.

2. The model

The model we shall consider is formulated so as to represent the wetting of a porous rock by two immiscible fluids, in the same way that conventional (one-species) directed site percolation (DP) may be thought of as the wetting of porous rock by a single fluid. The rock is modelled as a lattice of two types of pores, so that at each site there is either a large pore (probability p), a small pore (probability $r \leq 1 - p$) or a void (no pore). Two types of particle—small A-particles and large B-particles—are then allowed to infuse into the rock. The pores have the property that a large pore can accommodate a small or a large particle, whilst a small pore can only accommodate a small one.

We consider a d -dimensional semi-infinite geometry, with the free surface in contact with a reservoir of A- and B-particles. The surface layer is then randomly occupied by A- and B-particles. The sites on the layer next to the surface are then occupied according to the occupancy of the 'parent' sites (i.e. its nearest neighbour sites on the surface layer). A given site can only be occupied by an A-particle if one of its parent nearest neighbours is occupied by an A-particle (and similarly for B-particles).

These sites then act as parent sites for the second layer from the surface, which are occupied accordingly, and so on. The occupancy of a given site is therefore determined by two parameters: (i) the pore type; and (ii) by the occupancy of its parent nearest-neighbour sites. The rules we use are the following:

- (i) If all the parent sites are unoccupied, or the site is a void, then the site is unoccupied.
- (ii) If the site is a small pore (i.e. can only accommodate an A-particle), then:
 - (a) if at least one of the parent sites contains an A-particle, then the site is occupied by an A-particle; and
 - (b) if none of the parent sites contain an A-particle, the site is unoccupied.
- (iii) If the site is a large pore (can accommodate either type of particle), then:
 - (a) if all of the parents are unoccupied, the site is unoccupied;

- (b) if at least one parent site contains an A-particle, and none contain B-particles, the site is occupied by an A-particle;
- (c) if at least one parent site contains a B-particle, and none contain A-particles, the site is occupied by an B-particle;
- (d) if at least one parent site contains an A-particle and at least one contains a B-particle, then the site is occupied by a B-particle with probability α and an A-particle with probability $(1 - \alpha)$.

In the final case, where the occupancy of the site is determined by competition between the species A and B, we have introduced a parameter α , which represents the affinity of a large pore for the large B-particles. We shall find that the value of α , as well as the probabilities p and r , crucially affects the steady-state phase of the system.

The model may be mapped onto a three-state probabilistic cellular automaton, with $(d - 1)$ spatial dimensions and one 'time' direction (representing the direction in which the fluids infuse into the rock). In accordance with this representation, we shall always refer to the direction of percolation in this system as 'time' t , and to the state of the system as the occupancy of the t th layer. The state at a given site x at time-step $t + 1$ is a function of the site's neighbours at time t only. The site variable takes the values 0, 1, 2, representing an unoccupied site, a site occupied by an A-particle, and a site occupied by a B-particle respectively. For the rules described above, the occupancy of a given site is a function of whether there is *any* particle of a given type in the parent sites, and not on the total numbers (provided at least 1). This particular choice of rules is particularly convenient for the numerical simulation of this model, as the configuration of parent occupancies may be represented by an bitwise OR function. The cellular automata rules are defined in the table 1. $N(1)$ and $N(2)$ are the number of 1s and 2s in the parent sites, and $p(0)$, $p(1)$, $p(2)$ are the probabilities that the site will take the value 0, 1, 2 respectively.

Table 1. Probabilities of daughter state as a function of parent states. For notation, see text.

$N(1)$	$N(2)$	$p(0)$	$p(1)$	$p(2)$
0	0	1	0	0
≥ 1	0	$1 - (p + r)$	$p + r$	0
0	≥ 1	$1 - p$	0	p
≥ 1	≥ 1	$1 - (p + r)$	$r + p(1 - \alpha)$	αp

The model is very closely related to DP. In the absence of A-particles, the system behaves as DP in the B-particles with probability p , whereas in the absence of Bs (either by boundary conditions or by choosing $p = 0$), the As percolate with characteristic probability $(p + r)$. If there are no A-particles at time t , there are none at time $t' > t$ (and similarly for Bs); in particular, the state where there are neither As nor Bs is absorbing. The system may therefore be capable of evolving into several possible steady-states, depending on the initial conditions and the parameters α , p , and r . The steady-state is characterized by whether the A-particles, B-particles, or both species, may percolate and so survive with non-zero probability as $t \rightarrow \infty$.

Several cases may be discussed without calculation. For $p + r < p_c$ (where p_c is the critical probability for DP), neither species would be capable of percolating even in the

absence of the other, so the final state must always be the absorbing one. We assume that, for an infinite lattice with non-zero initial occupations of both species, if one species is not capable of percolating, then it will only survive for a finite characteristic time, and initial fluctuations in the densities will be sufficient to ensure that its initial presence will not affect the ultimate survival of the other species. For $p < p_c$, the B-particles are never capable of percolating, so the region $p + r > p_c$, $p < p_c$, must be characterized by a steady-state with the As obeying DP, the line $p + r = p_c$ being a line of second-order DP transitions.

For $\alpha = 1$, all competition processes are 'won' by B-particles. Thus, the Bs percolate completely independently of the As. Hence, in this case, the density of B-particles in the final state undergoes a conventional DP transition along $p = p_c$. The question of whether a non-zero density of As may exist in this state may not be answered without further calculation. Similarly, in the case $\alpha = 0$ the A-particles always follow DP, though it may still, in principle, be possible to obtain a phase with non-zero B-particle density as well.

If there exist steady-state phases with non-zero concentrations of both species, the order of transitions between such phases is not evident *a priori*. The fluctuations in the density of one species may be expected to influence in a relevant way the fluctuations in the other species, and so it is likewise not clear *a priori* whether any second-order transitions will be in the universality class of DP.

3. Mean-field analysis

In this section, we analyse the system within the framework of a simple mean-field theory approach. This is expected to reproduce qualitatively correct phase diagrams, at least in high dimensions, although the critical exponents are not expected to be determined accurately.

We characterize the state of the system simply by its average densities $n_A(t)$ and $n_B(t)$ of the A- and B-particles at the t th time-step. The density of unoccupied sites is then $n_0(t) = (1 - n_A(t) - n_B(t))$. The probabilities $n_A(t + 1)$, $n_B(t + 1)$ that a site at time-step $(t + 1)$ is occupied by an A- or B-particle are then related to the probabilities that the parent sites at time t contain zero or non-zero numbers of each of the two species. Let $P_{0,0}$ be the probability that the parent sites contain neither A- nor B-particles, $P_{\geq 1,0}$ be the probability that at least one of the parent sites contain an A but no sites contain Bs, etc. Then the equations of motion for the densities are, according to the probabilities in table 1,

$$n_0(t + 1) = P(0, 0) + [1 - (p + r)]P_{\geq 1,0} + [1 - p]P_{0,\geq 1} + [1 - (p + r)]P_{\geq 1,\geq 1} \quad (1)$$

$$n_A(t + 1) = (p + r)P_{\geq 1,0} + [r + p(1 - \alpha)]P_{\geq 1,\geq 1} \quad (2)$$

$$n_B(t + 1) = pP_{0,\geq 1} + p\alpha P_{\geq 1,\geq 1}. \quad (3)$$

The mean-field assumption is that the probabilities P are related simply to the mean particle densities at the time-step t . If the lattice is such that each site has $z(\geq 2)$ parent sites, then (for instance) the probability that no parent sites contain B-particles is just $(1 - n_B)^z$. The P are then given, in mean-field theory, by the

following equations:

$$P_{0,0} = n_0^z(t) \tag{4}$$

$$P_{\geq 1,0} = [1 - n_B(t)]^z - n_0^z(t) \tag{5}$$

$$P_{0,\geq 1} = [1 - n_A(t)]^z - n_0^z(t) \tag{6}$$

$$P_{\geq 1,\geq 1} = 1 - P_{\geq 1,0} - P_{0,\geq 1} - P_{0,0}. \tag{7}$$

Substituting (4)–(7) into (1)–(3), the mean-field equations for n_A , n_B are most conveniently written in the following form.

$$n_A(t + 1) = (p + r)[1 - \{1 - n_A(t)\}^z] - p\alpha[1 - \{1 - n_A(t)\}^z - \{1 - n_B(t)\}^z + \{1 - n_A(t) - n_B(t)\}^z] \tag{8}$$

$$n_B(t + 1) = p[1 - \{1 - n_B(t)\}^z] - p(1 - \alpha)[1 - \{1 - n_A(t)\}^z - \{1 - n_B(t)\}^z + \{1 - n_A(t) - n_B(t)\}^z]. \tag{9}$$

The evolution of the system is obtained by iterating equations (8) and (9). The steady-state solutions are obtained by setting $n_{A(B)}(t + 1) = n_{A(B)}(t)$ in (8) and (9). Although several steady-state solutions may exist, they may be either stable or unstable to small perturbations in the initial value of the densities; this stability is exactly the same as the stability of the iteration of the above equations. The first term in both equations (8) and (9) is that which would be present for DP of one species in the absence of the other. The second term is always negative, being zero if either $n_A(t)$ or n_B is zero. Therefore, the steady-state values of the two densities must always be less than or equal to their DP values in the absence of the other species.

The simplest case to discuss is when $\alpha = 1$. Here, from equation (9), n_B is independent of n_A and so assumes its DP value. There is, therefore, a second-order phase transition in n_B along the line $p = p_c (= 1/z)$, such that the B-density behaves as

$$n_B \simeq \frac{2z}{z - 1}(p - p_c). \tag{10}$$

near the transition, i.e. the critical exponent is unity. The A-density n_A assumes its DP value for $p \leq p_c$. For $r > 0$, $n_B = 0$, the solution to (8) is stable to infinitesimal perturbations in n_B and changes linearly in δp . The line $p = p_c$ is therefore a line of second-order phase transitions from a phase containing only A-particles (henceforth ‘A-phase’) to a phase containing both A- and B-particles (henceforth ‘AB-phase’).

As p (and therefore n_B) increase, however, the second term in equation (8) causes the value of n_A to decrease monotonically. For a given value of r , there is a critical value p'_c of p at which the only steady-state value of n_A is zero, and above which the solution $n_A = 0$ is stable. This value is the point where the gradient of the right-hand side of (8) becomes equal to unity for $n_B = 0$, i.e.

$$1 = (p'_c + r)z - p'_c z (1 - (1 - n_B)^{z-1}) \tag{11}$$

where n_B assumes its DP value. Tedious algebra shows that dr/dp'_c decreases monotonically with p . Substituting from (10) gives the gradient of the phase boundary at $p = p_c$

$$\left. \frac{dr}{dp'_c} \right|_{p=p_c} = 1. \quad (12)$$

For $\alpha \neq 1$, the situation is more complicated. However, it is still the case that there exists only one stable solution for given p , r , α . To see this, consider the coupling term (the coefficient of αp in (8)). The absolute value of this term increases monotonically as a function of both n_A , n_B , and so if the solution with n_A (or n_B) is stable, there is no other stable point. Similarly, if there is a solution with both n_A , n_B non-zero, this point must be stable and the origin is unstable. All phase transitions are therefore of second order, and the phase boundaries are given by the points where either n_A or n_B become marginally stable at the origin. Since a linear perturbation in p or r always produces a linear change in the densities, the critical exponent is always unity, i.e. it is in the universality class of directed percolation (within mean-field theory). The boundary of the A/AB-phase transition is therefore given by

$$1 = zp - zp(1 - \alpha)[1 - \{1 - n_A\}^{z-1}] \quad (13)$$

$$n_A = (p + r)[1 - \{1 - n_A\}^z] \quad (14)$$

and the boundary of the B/AB-phase transition by

$$1 = z(p + r) - zp\alpha[1 - \{1 - n_B\}^{z-1}] \quad (15)$$

$$n_B = p[1 - \{1 - n_B\}^z]. \quad (16)$$

These phase boundaries have the following properties:

(1) *A/AB boundary*: The gradient of the phase boundary increases monotonically with p , and at $p = p_c$ has the value

$$\left. \frac{dr}{dp} \right|_{A/AB, p=p_c} = \frac{2\alpha - 1}{2(1 - \alpha)}. \quad (17)$$

At the value $\alpha = \frac{1}{2}$, this gradient is zero, and for $\alpha < \frac{1}{2}$, the boundary intercepts the $r = 0$ axis at some value $p > p_c$. The boundary intercepts the line $(p + r) = 1$ at $p_{A/AB} = 1/\alpha z$, where the gradient is

$$\left. \frac{dr}{dp} \right|_{A/AB, p+r=1} = \infty.$$

For $\alpha < \frac{1}{z}$, there is no AB-phase at all.

(ii) *B/AB boundary*: The gradient of the boundary decreases monotonically with p , and at $p = p_c$ assumes the value

$$\left. \frac{dr}{dp} \right|_{B/AB, p=p_c} = 2\alpha - 1. \quad (18)$$

For $\alpha < \frac{1}{z}$, this phase does not exist at all. The boundary has an intercept with $(p + r) = 1$ if $z > 1/(1 - \alpha)$, intercepting at $p = 1$ for $\alpha = (z - 1)/z$.

The phase diagram for $z = 4$ is shown from a numerical evaluation of equations (13)–(16) in figure 1 for $\alpha = 0.3, 0.5, 0.75, 1.0$. The features discussed above are clearly present. Qualitative features of the diagram are insensitive to the value of z .

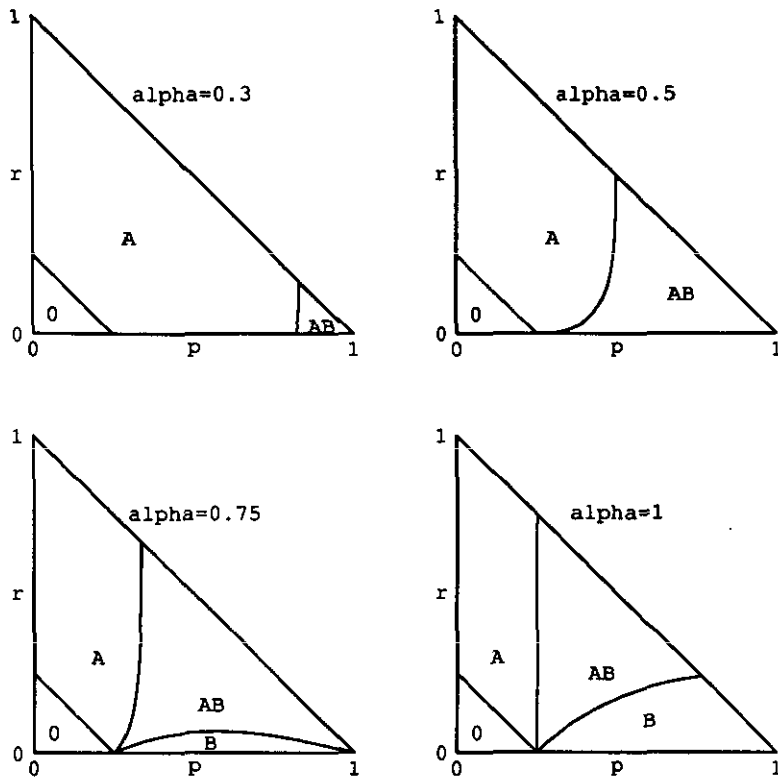


Figure 1. Mean-field phase diagrams for $z = 4$ and $\alpha = 0.3, 0.5, 0.75, 1.0$ respectively. For this value of z , the percolation threshold is $p_c = 0.25$.

4. The true phase diagram

The mean-field analysis in the previous section predicted that all phase transitions in this system are of second order. Within mean-field theory, the critical exponent is always the same for all transitions, since the changes in the densities are always linear at the boundaries.

In order to investigate the true behaviour, we performed simulations of the probabilistic CA rules in table 1 in dimensions $1 + 1$ and $2 + 1$. To determine the phase diagram, between 10 and 30 independent realizations of the system were allowed to evolve for between 2000 and 20 000 time-steps. Typical lattice sizes were 256 in dimension $1 + 1$ and 64×64 in dimension $2 + 1$. For points well away from the phase boundaries, the system quickly settled into one given steady-state. Near the phase boundaries, large fluctuations allowed the system to settle into either of the two possible stationary states, and so large samples and long times were needed to distinguish the state of the system. Near $r = 0$, and for $\alpha \approx \frac{1}{2}$, it takes a long time for the one species to be favoured over another because the competition between the two species is very close, and so it was difficult to evaluate the phase diagram with accuracy.

4.1. $d = 1 + 1$

For dimension $1 + 1$, no steady-state may exist with non-zero densities for both A and B. This can be seen from topological arguments, since it is not possible to construct two

different but intersecting percolation clusters in this dimensionality. For this reason, there exists no AB-phase for $d = 1 + 1$. The line $p + r = p_c$ is still a second-order line to the A-phase. For $p < p_c$ only the A-phase can be stable, with n_A assuming its DP value (with characteristic probability $p + r$). In the B-phase n_B must assume its DP value with characteristic probability p . For $\alpha < \frac{1}{2}$, competition processes tend to favour the A-particles, which also have higher percolation probability, and so there exists no phase transition to a B-phase. For $\alpha = \frac{1}{2}$, A-particles are always favoured for $r > 0$, whilst along the line $r = 0$, A and B are equivalent and so we can have either the A- or B-phase; domains of the two phases will grow indefinitely with time.

For $\alpha > \frac{1}{2}$, n_A must always change discontinuously across the transition, and so the transition is first order. For $\alpha = 1$ (only), the B-particles percolate independently of the As, and so the phase boundary is the line $p = p_c$; in this case, n_B has a second-order phase transition along this line, within the universality class of directed percolation.

Figure 2 shows the phase diagram obtained from simulations of the system in $d = 1 + 1$ for $\alpha = 0.7, 1.0$. The A/B-phase transitions appear to be unambiguously first order, to within the accuracy of the simulations. The uncertainty in the position of any given point on the transition lines is typically of the order of ± 0.005 .

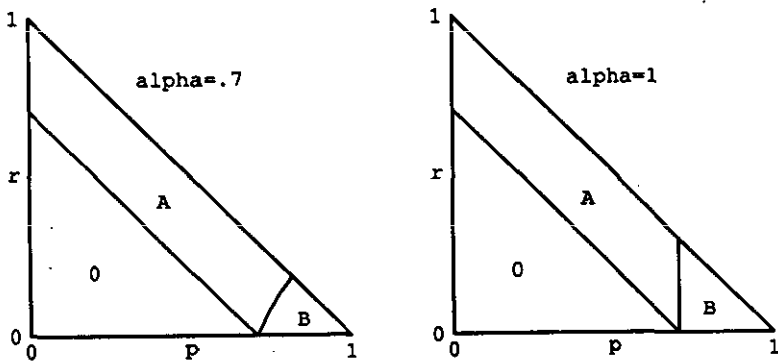


Figure 2. Phase diagrams for $d = 1 + 1$, and $\alpha = 0.7, 1.0$.

4.2. $d = 2 + 1$

In higher dimensions than $1 + 1$, two independent interlocking percolation clusters can coexist, and so the topological arguments in the previous subsection do not apply. Several features of the phase diagram may still be obtained exactly, however. Firstly, the threshold for the the A-phase occurs at $p + r = p_c$, and for $\alpha = 1$ the A/AB-phase transition line is always at $p = p_c$. For $\alpha < \frac{1}{2}$, there can be no pure B-phase.

Certain other features that would be expected but about which there are no rigorous arguments are reproduced by the simulation results. Figure 3 shows the phase diagrams for a body-centred cubic lattice, for the values $\alpha = 0.4, 0.5, 0.6, 1.0$. For this lattice, the threshold for DP is $p_c = 0.3445 \pm 0.00012$ [6]. For $\alpha = \frac{1}{2}$, the A/AB transition line has zero gradient at $p = p_c$, whilst for $\alpha < \frac{1}{2}$ the threshold for the A/AB transition is at $p > p_c$.

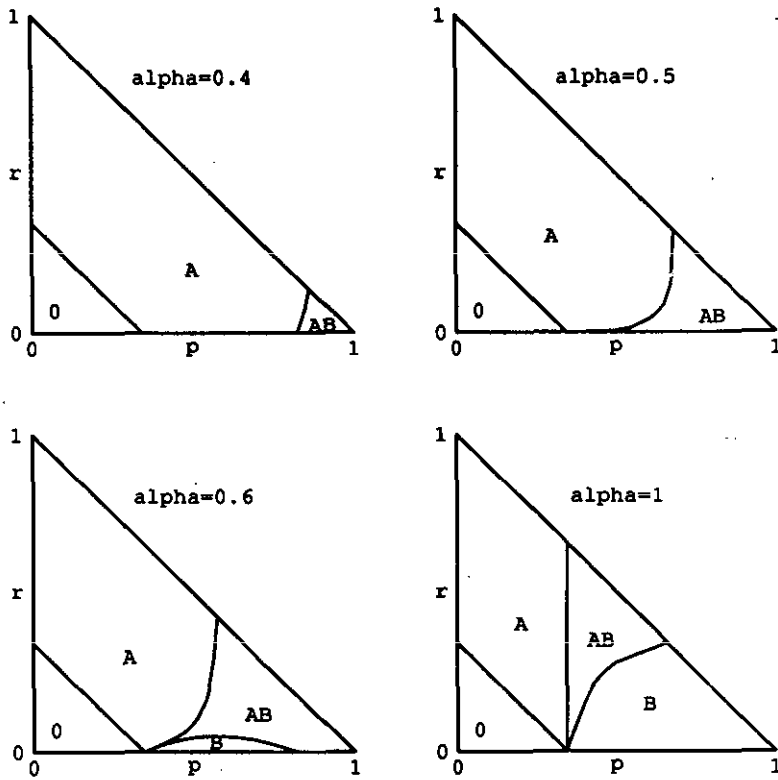


Figure 3. Phase diagrams for $d = 2 + 1$ and $\alpha = 0.4, 0.5, 0.6, 1.0$.

5. Critical exponents

According to the arguments presented in the previous section, in dimension $d = 1 + 1$ the transitions are either of first order or are simple DP transitions. In dimension $d = 2 + 1$ the situation is much less clear. There are second-order transitions to phases with non-zero concentration of both A and B which arise due to competition between species. We therefore turn to simulations to determine the universality classes of these transitions.

The transition could be investigated at any point along one of the transition lines. We choose to investigate the case $\alpha = 1$ at the point of intersection of the AB/B transition with the line $p + r = 1$. The simulation can be coded in a more efficient way along the line $p + r = 1$, which therefore reduces the CPU time necessary.

We follow the method used previously by Grassberger to investigate the critical exponent of the DP case in $d = 2 + 1$ dimensions [6]. We start with a lattice filled with B-particles with one site containing an A-particle. The system is allowed to evolve according to our CA rules. We measure the density $n_B(t)$, the average square cluster size $R^2(t)$ and the survival probability $P(t)$ during the simulation. The system is sufficiently large that none of the clusters we simulated reached the boundaries, and so our data are free of finite size effects. These simulations take more time than those for DP, since we have to keep track of both species. More averages would be necessary to reduce the noise in the figures. Each line corresponds to an average over 24 000 independent evolutions, and required 20 h on an IBM 3090.

At the critical point, we expect asymptotic power-law evolution, described by the following equations

$$n_B(t) \sim t^\eta \quad (19)$$

$$R^2(t) \sim t^z \quad (20)$$

$$P(t) \sim t^{-\delta}. \quad (21)$$

These three quantities are plotted as a function of time on a log-log scale in figures 4, 5 and 6. $n_B(t)$ is the average over all clusters (including those which have already died out), while R^2 is averaged only over surviving clusters. Five values of p are shown; upward (downward) curvatures indicate that the A-species is super (sub) critical. This leads to the estimate $p_c = 0.66825(10)$. Our best estimates for the exponents are:

$$\eta = 0.220(17) \quad z = 1.115(35) \quad \delta = 0.444(20). \quad (22)$$

These values are compatible with the accepted DP results ($\eta = 0.214(8)$, $z = 1.134(4)$, $\delta = 0.460(6)$). There is therefore no evidence that the phase transition is in a different class from DP.

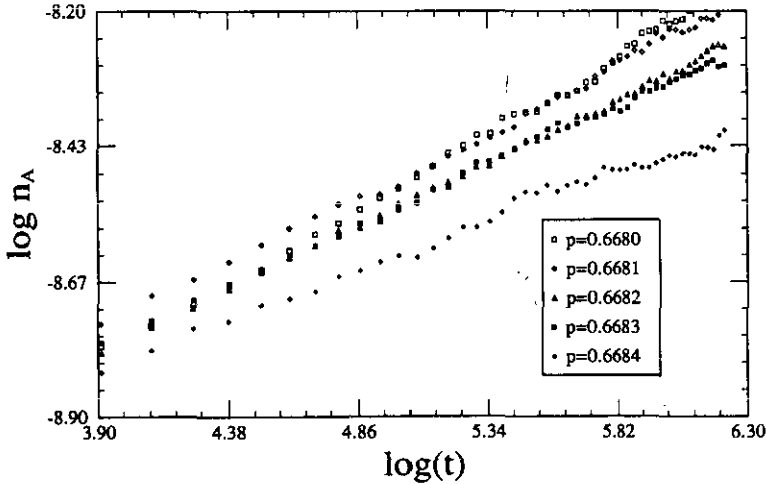


Figure 4. Density of the A-species as a function of time for five values of p , on a log-log scale.

6. Conclusions

The model we have studied possesses a very rich phase diagram, with phase transitions induced by the competition between the two species as well as by simple percolation. The mean-field theory of this system has predicted phase diagrams which are in good qualitative agreement with our simulations in dimension $d = 2 + 1$, whilst in dimension $d = 1 + 1$ a line of first-order transitions is predicted by topological arguments and reproduced by simulations. It appears, however, that (at least at the point we investigated) the critical exponents in this system fall within the universality class of

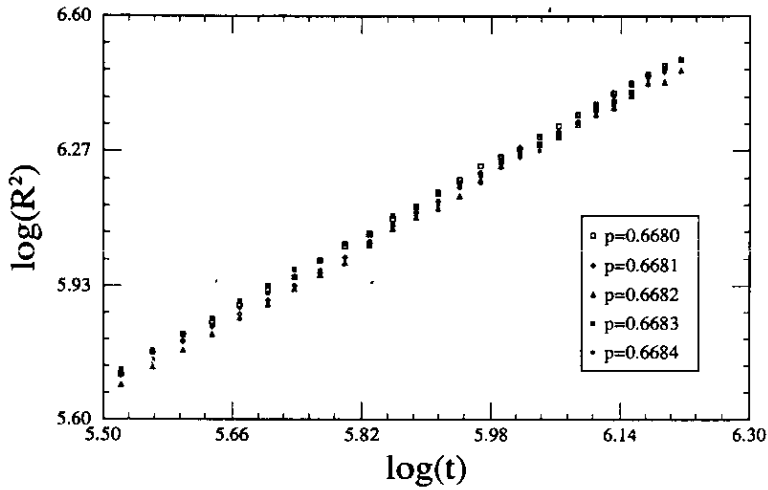


Figure 5. The mean-square cluster radius R^2 , as a function of time, on a log-log scale.

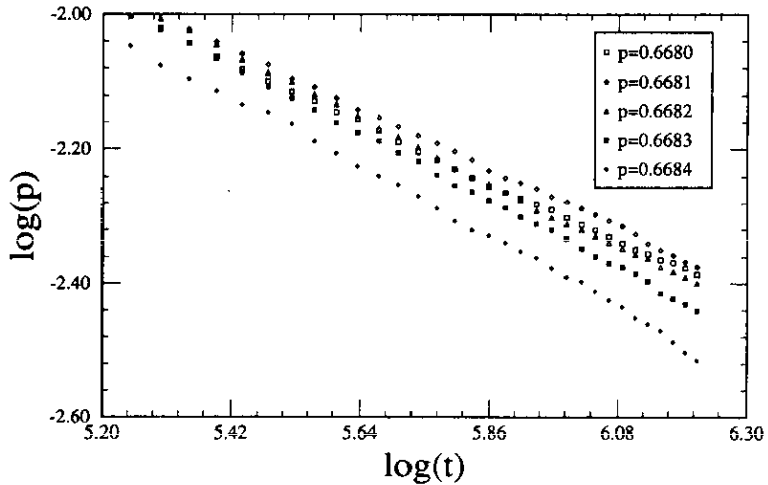


Figure 6. Survival probability P as a function of time, on a log-log scale.

conventional directed percolation. More simulations at different points are required to verify this, however, and this question is currently under investigation.

Several other aspects of this model deserve further study, however. In contrast to DP, it is possible to study interfaces in this model. The growth of domains of the A- and B-phases at the coexistence line would be expected to display a new dynamic scaling behaviour. The scaling theory near the multicritical point $p = p_c$, $r = 0$ is also expected to be subtle.

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