Percolation of randomly distributed growing clusters: the low initial density regime

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Received 10 November 2010 / Received in final form 11 April 2011
Published online 25 May 2011 – © EDP Sciences, Società Italiana di Fisica, Springer-Verlag 2011

Abstract. We investigate the problem of growing clusters, which is modeled by two dimensional disks and three dimensional droplets. In this model we place a number of seeds on random locations on a lattice with an initial occupation probability, \( p \). The seeds simultaneously grow with a constant velocity to form clusters. When two or more clusters eventually touch each other they immediately stop their growth. The probability that such a system will result in a percolating cluster depends on the density of the initially distributed seeds and the dimensionality of the system. For very low values of \( p \) we find a power law behavior for several properties that we investigate, namely for the size of the largest and second largest cluster, for the probability for a spanning cluster to occur, and for the mean radius of the finally formed droplets. We report the values of the corresponding scaling exponents. Finally, we show that for very low initial concentration of seeds the final coverage takes a constant value which depends on the system dimensionality.

1 Introduction

Percolation theory has drawn a continuous interest from the scientific community for several years [1–6]. It has been studied in a wide variety of systems ranging from lattices [7] to complex networks [5,6]. The fields that percolation applies are as diverse as electromagnetism [8,9], chemistry [10], materials science [11], geology [12], social systems [13], wireless networks [14] and many more. In chemistry and materials science it is of major importance for the movement of liquids or gases in porous media. Problems in this area relate to the leakage in seals [15] and the gas permeability in cement paste [16].

Various algorithms have been used to simulate the phase transformation kinetics. In many pattern formation models several small spherical seeds are nucleated at a constant rate (homogeneous nucleation). Seeds can also initiate on defects in the case of heterogeneous nucleation. From the simulation point of view the defects are considered as points in the lattice representing the seeds. The seeds once formed are in a metastable phase and grow at a constant velocity as long as there is adequate available material for adsorption.

Additionally, several models exist that do not allow the adsorption of a new particle in contact with or overlapping with an already adsorbed one. An example is the random sequential adsorption (RSA) model [17]. This model has been extensively used for colloid and globular protein adsorption in heterogeneous surfaces. In such systems discrete lattice sites can act as adsorption sites with attractive short range interactions [18]. The jamming coverage and the structure of the particle monolayer as a function of the site coverage and the particle/site size ratio have been studied.

Models studying pattern formation ranging in between these two cases have not been used extensively. Andrienko proposed [19,20] the idea of disks and droplets growing at a constant rate on random initial sites over the lattice and stopping once they come in contact. In the so called “Touch and Stop” model the droplets grow at a constant rate in all directions (circular in 2D, spherical in 3D). The geometrical properties of emerging patterns, the growth kinetics and the fraction of untransformed material have been examined both by a mean field approach and Monte Carlo simulations.

The main characteristic of this model is located in the notion that the droplets stop growing after two or more of them come in contact. This can be due to several reasons. In material science it is possible to have a strong surface tension that inhibits the nuclei from taking any shape other than that of a circular or spherical one. Additionally, a significant interacting force between the substrate and the forming droplet can prevent two or more discs from coalescing in the time scale needed for the growth of other islands.

This problem relates to the well studied Apollonian packing problem [21] for circles and spheres. In fact it can be considered as a random version of packing with various discrete sizes, where growth velocity is constant but not infinitely large. The Touch and Stop model has also been
studied in some variations (random insertion of seeds in time) as a packing limited growth problem [22]. It is also related to the “cluster-cluster aggregation” model [23,24] and to continuum percolation problem [4]. In cluster-cluster aggregation particles are randomly placed on the lattice and considered to form clusters if they touch. Clusters are moved as a whole either with the same probability or with probability inversely proportional to their mass. One is mainly interested in the time needed for a giant component to emerge. In the model of continuum percolation, discs of a certain radius are randomly placed on a two dimensional surface creating clusters of overlapping discs [4]; page 54. The continuum percolation model is known to belong to the same universality class as lattice percolation.

2 Model description

The system used can be described as follows. Initially, lattices of $10^6$ sites ($1000 \times 1000$ for 2D, and $100 \times 100 \times 100$ for 3D) are randomly populated with seeds of singular size in a non overlapping way. The initial occupation probability of these sites is $p$. At every time step all seeds are investigated once as to the possibility of growing in size instantaneously in all neighboring sites. Investigation sequence is random in order. Each seed is allowed to grow its periphery by one layer (increase the radius by one) provided that there is no overlapping with other growing seeds. Thus each seed becomes an evolving cluster. As soon as two, or more, clusters touch each other, the growth of all of the adjoined clusters stop. Such an assumption is justified in systems where there is high surface tension which causes homogeneous cluster growth. The touching disks or droplets can be considered as belonging to the same stable cluster, a cluster that no longer grows over time unless other evolving clusters happen to touch it. Periodic boundary conditions are applied in both the 2D and 3D systems. In order to ensure a smaller statistical error a large number of runs was used (1000 individual configurations).

The system continues to evolve until no other cluster can grow in time, so that all of them have at least one adjoining cluster. At this point the final occupation probability of each site is generally larger than $p$ and the system is investigated as to whether it has a spanning cluster using the classic Hoshen-Kopelman algorithm [25]. The final shape of each disk or droplet of this system is not circular or spherical, in 2D and 3D. It is square and cubic, respectively. Therefore, it is possible that two evolving clusters have more than just one adjoining sites. In order to have only one adjoining site they must touch at their tips. When two such clusters touch in a part of one of their edges (2D) or facets (3D), the resulting stable cluster formed has two clusters which are connected in more than just one site. Snapshots of a typical finite 2D system evolution can be seen in Figure 1, and a larger snapshot of the final state of a system with very low concentration of initial seeds is given in Figure 2. It is obvious in Figure 2 that several clusters are connected in two or more sites.

3 Discussion

Starting from an empty lattice, we vary $p$ in the entire domain $0 < p < 1$, allow the system to evolve, and we monitor the size of the largest, $S_1$, and second largest, $S_2$, clusters formed in the final stable configuration (Figs. 3 and 4). In contrast to the classical percolation model where small concentrations of seeds translates to either isolated sites or very small formed clusters, our model exhibits at first high values for the normalized sizes of the two largest clusters. For low concentrations, the values of $S_1$ and $S_2$ are quite large. This can be explained by the very small number of initial seeds in our system which means that they are randomly placed far apart from one another. This enables them to grow without touching each other for many time steps. Therefore, the largest clusters end up with a high final size value.

In fact, if we simply have one initial seed, then that one also forms the spanning cluster. This is obviously a finite size effect and is due to the periodic boundary conditions applied. This will cause the growing droplet to eventually touch itself on two opposite vertices of the evolving cluster.

![Fig. 1. (Color online) Snapshots of the evolution of a 2D system. Each snapshot corresponds to an advance of 1 time unit. The first snapshot is the initial system and the last is the final system configuration, where no percolating cluster is formed. Different colors signify different evolving clusters. At snapshot 4 the evolution of the blue and red droplets stops since they touch and the blue and red droplet now form one stable cluster. All other clusters stop growing at snapshot 5. Periodic boundary conditions are used.](image1)

![Fig. 2. (Color online) Snapshot of the final state of a 2D 500×500 system with very low concentration of seeds ($p = 0.001$). Each stable cluster has a different color and the largest is shown in black.](image2)