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Properties of percolation clusters in a model granular system in two dimensions

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Abstract. Properties of percolation clusters in a model granular system on a square lattice are examined by a Monte Carlo simulation. Grains are grown around seeds up to the nth neighbours. The critical coverage at the percolation threshold is shown to oscillate as a function of n. The fractal dimension and critical exponents are shown to be compatible with those of the standard percolation process.

1. Introduction

Granular materials are among non-crystalline solids which have been extensively studied in recent years because of their practical importance [1]. Characterization of the structure of granular systems is one of the most important steps towards understanding their properties. The connectivity and the distribution of clusters are among the most important properties which can be analysed by the percolation theory.

A grain can be considered to consist of some number of particles, and thus the granular percolation can be regarded as a special case of correlated percolation [2]. It is known that correlation in particle distribution changes the percolation properties [3]; while moderate attractive interaction reduces the percolation threshold, much stronger attraction between particles increases it [2].

In this paper we generalize the basic concept of percolation theory and apply it to a model granular system in two dimensions. We consider a specific correlation of particle distribution, where particles are assumed to form a definite grain with the same shape, and study the effects of the shape of grain on percolation properties. Monte Carlo simulation is exploited to study the critical percolation coverage and various properties of clusters as functions of the size of grains. In particular, it is shown that the critical percolation coverage oscillates as a function of the size of grains and that the critical exponents are compatible with the universal value for the standard percolation. In section 2, we explain our model granular system. We show the results of our simulation in section 3, where the critical percolation coverage, the fractal dimension and the critical exponents are studied. Results are discussed in section 4 and conclusions are given in section 5.

2. Model granular system

We distribute seeds randomly on a square lattice (500×500, except for the simulation related to the finite size scaling) with a given concentration, p_i. Each seed is then grown

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up to the nth neighbours, where overlap of grains is allowed. Figure 1 shows grains for $n = 4, 5, 6, 7, 8$. (See figure 5 for examples of the model granular system.) The coverage of the system is defined by the fraction of occupied sites and is denoted by p_g. Note that p_g corresponds to the occupation probability in the standard percolation process.

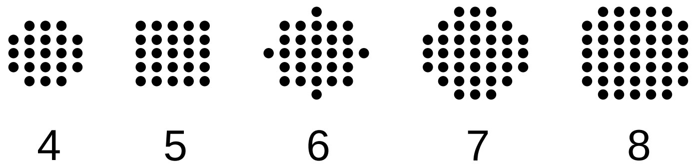


Figure 1. Grains for the 4th–8th generation which are grown from the seed at the centre.

We connect particles occupying adjacent neighbour sites and construct clusters by mutually connected particles. The percolation is judged by the existence of a cluster spanning all sides of the system. We denote the critical percolation seed density and coverage by $p_i^C(n)$ and $p_g^C(n)$, respectively.

At the percolation threshold, the size ('mass'), S, of the percolating cluster within radius r is scaled as

$$S \sim r^{d_f} \tag{1}$$

which defines the fractal dimension d_f [4]. We also introduce the critical exponents β, γ and ν for the percolation probability, the mean cluster size and the correlation length in the same fashion as in the standard percolation process [4].

3. Results

3.1. Critical percolation coverage

We determined $p_i^C(n)$ and $p_g^C(n)$ for each of 100 different runs and the average of them with standard deviation is listed in table 1. Figures 2(a) and (b) show the dependence of $p_i^C(n)$ and $p_g^C(n)$ on the generation of the grain. We see that while the critical seed density is a monotonically decreasing function of n, the critical coverage oscillates as a function of n.

Table 1. Critical percolation coverage $p_g^C(n)$ and critical percolation seed density $p_i^C(n)$.

n	$p_g^C(n)$	$p_i^C(n)$
0	0.594 ±0.004	0.594 ±0.004
1	0.586 ±0.007	0.162 ±0.003
2	0.596 ±0.009	0.0958 ±0.002
3	0.610 ±0.009	0.0699 ±0.002
4	0.625 ±0.011	0.0456 ±0.001
5	0.618 ±0.013	0.0378 ±0.001
6	0.605 ±0.012	0.0316 ±0.001
7	0.639 ±0.014	0.0272 ±0.001
8	0.637 ±0.014	0.0223 ±0.0008
9	0.625 ±0.014	0.0198 ±0.0008
10	0.639 ±0.015	0.0177 ±0.0008

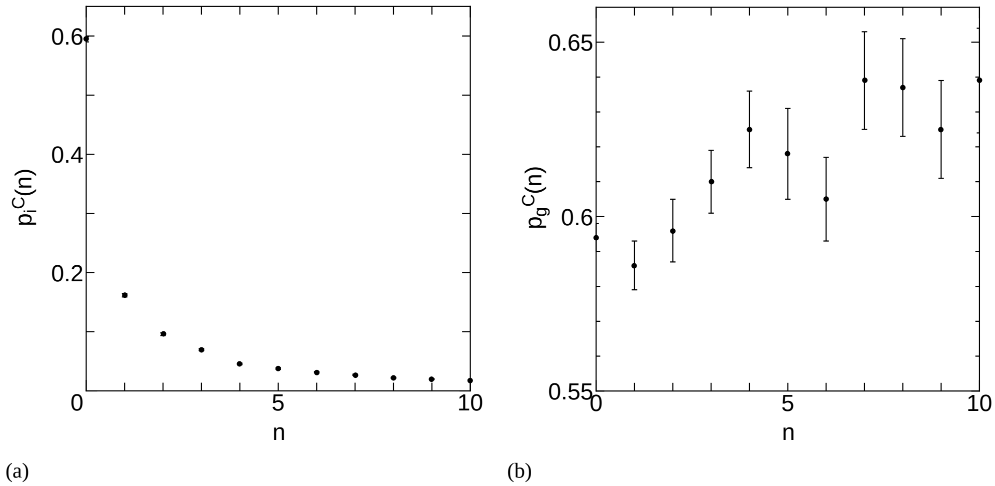


Figure 2. (a)The critical percolation seed density $p_i^C(n)$ and (b) the critical percolation coverage $p_g^C(n)$ are plotted against n. Although $p_i^C(n)$ is a monotonically decreasing function of n, $p_g^c(n)$ oscillate as a function of n. (Error bars in (a) are within the size of the circles.)

3.2. Fractal dimension and other critical exponents

We employed the standard box counting method to determine the fractal dimension d_f at the percolation threshold which is shown in figure 3. For the grain sizes studied here, the fractal dimension does not depend on the generation of grains.

With the use of the finite size scaling method, we also determined the critical exponents β/ν and γ/ν for the percolation probability and the mean cluster size. We test in figure 4

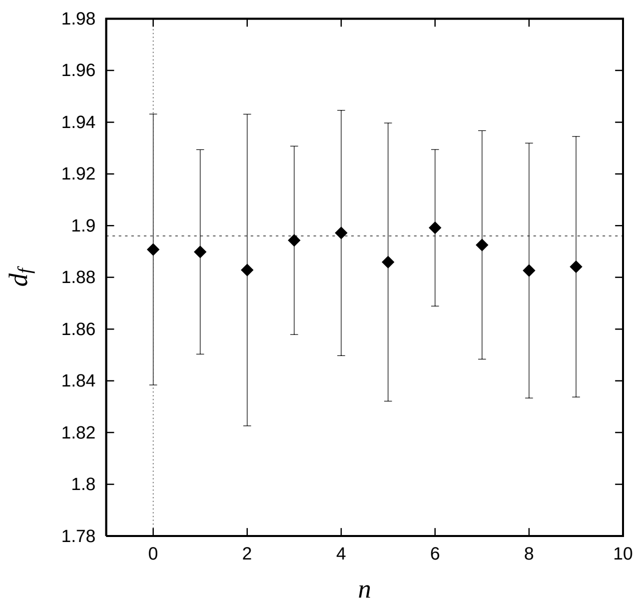


Figure 3. The fractal dimension is plotted against n.

the hyperscaling relation between them

$$2\beta/\nu + \gamma/\nu = 2, \tag{2}$$

by plotting the left-hand side against n. Within the error bars, the scaling relation (2) holds for the grains studied here.

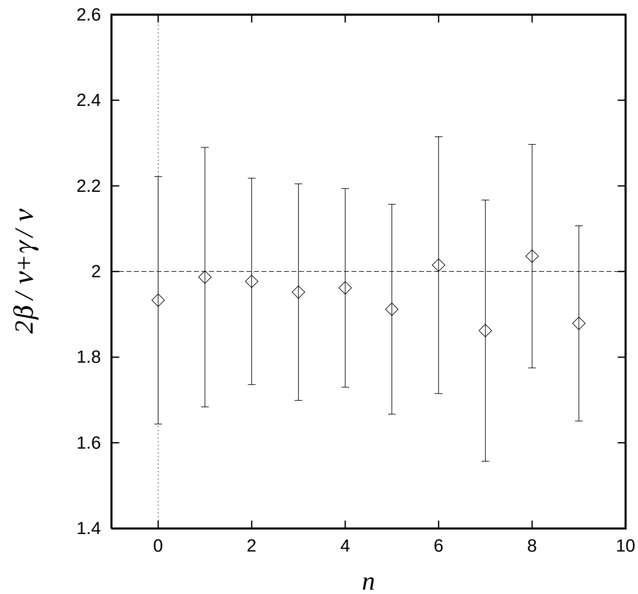


Figure 4. Test for the hyperscaling relation $2\beta/\nu + \gamma/\nu = 2$ for various n.

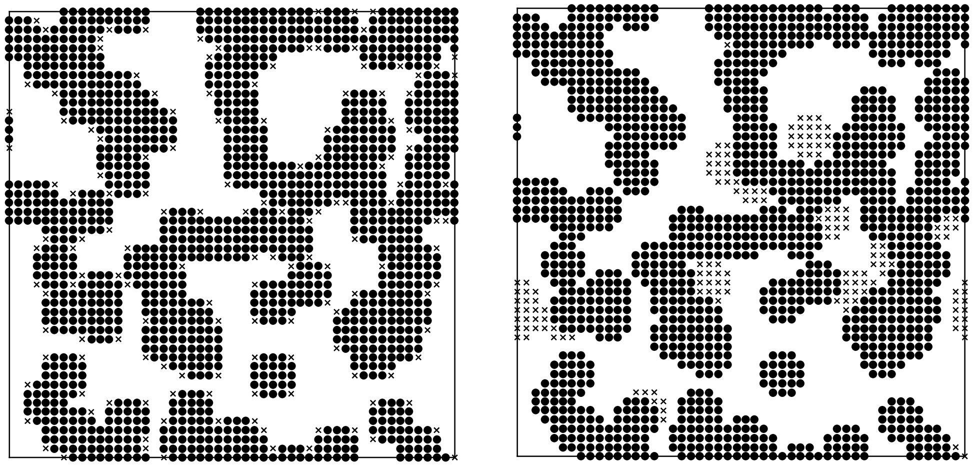
4. Discussion

First, we notice, in figures 2(a) and (b), that $p_i^C(0) = p_g^C(0)$ is about 0.594 which agrees with the well known critical percolation concentration for the site process of the square lattice [4]. Secondly, we note that $p_g^C(n)$ shows oscillation with minima at $n = 1, 6, 9$. This indicates, for example, that the connectivity for grains of the 5th generation is larger than that of the 4th generation, To see this effect, we compare systems with the same coverage in figure 5, where cosses in figure 5(a) are moved to form $n = 5$ grains in figure 5(b). While there exists a percolation path in figure 5(a) for $n = 4$ grains, the percolation path is lost in figure 5(b) for $n = 5$ grains even though the coverages are the same.

We can see in figure 3 that the fractal dimension is close to 1.896, the value for the standard process, and does not seem to depend significantly on the generation of grain at least for $n \leqslant 9$. As we have shown elsewhere [5], the critical exponent, ν, of the correlation length is also very close to the value for the standard process. The critical exponents β/ν and γ/ν also seem to satisfy the scaling relation (2) at least for $n \leqslant 9$ as one can see in figure 4.

5. Conclusions

First, we note that although granular materials are mostly grown on a crystalline substrate, they are among non-crystalline solids since they do not possess any translational symmetries.



(a) (b)

Figure 5. A part of the model granular system at the coverage $p_g \sim 0.607$ which is larger than $p_g^C(0) = 0.594$. (a) The 5th generation grains, where there is a channel connecting the right and left edges. ($\bullet$ and $\times$ have no differences.) (b) The 4th generation grains, where the connectivity is lower than in (a). Note that (b) is produced by removing $\times$'s in (a) and redistributing them as grains of the 4th generation.

The model system we studied in this paper well represents characteristics of granular materials, though the orientation of grains is restricted in the model system.

The connectivity of grains plays a major role in determining transport properties. In fact, Makhlouf *et al* [6] showed that the giant magnetoresistance of a granular material consisting of a magnetic atom and a non-magnetic metal may be attributed to scattering by the surface atoms. Therefore, it is important to construct a concept for granular materials which is utilized for the analysis of the connectivity.

In this paper we investigated the percolation process in the model granular system and found that:

(i) The critical percolation coverage oscillates as a function of the generation of grains. We have examined the connectivity near the minima of the plot $p_g^C(n)$ vs n and conclude that the projections of a grain are responsible for the increased connectivity for the grains of the 1st, 6th and 9th generations.

(ii) The fractal dimension and the critical exponents are consistent with the universal value.

We thus conclude that the shape of grains plays a role in determining the critical percolation coverage. This result indicates that granular materials may have properties significantly different from systems consisting of particles with simple attractive interaction between them.

Acknowledgments

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