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Wall effects on the percolation of small grains in 2D ensembles

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Abstract

This work studies the dependence of percolation properties of bidimensional arrays of polydispersed disks on the distance separating the walls of the container holding them. Data for percolation probabilities using different wall separation is analyzed for two extreme values of polydispersity. Conclusions on the effect that the container width has on the behavior of those properties are presented and discussed.

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1. Introduction

Arrays of solid particles are physical systems representing many basic and technological problems in granular matter field. They present the beauty and "apparent" simplicity of familiar situations but, at the same time, offer the complexity of a many body problem without exact solutions.

From pharmaceutical to mining engineering processes, all scales of grains and containers holding them are implied, with lots of operating setups and with needs of a good characterization in order to optimize mixing, transport and packing of the

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particles. Many works have attended the above-mentioned problems and much progress have been done in this direction but there are still many questions to answer [1–8].

Ippolito et al. [5] studied the dispersion properties of individual spherical small particles moving under gravity in a random packing of large spheres of diameter D. They analyze dispersion in the direction parallel and transverse to the mean velocity by studying the beads distribution in the x–y plane at the exit of the packing, while varying the height of the bed. Diffusion behavior was found in both directions and the dispersivity length was determined. They found that the path length was controlled by the diameter of the large beads, and that the dispersivity length increased with D, the diameter of the beads in the packing. Cooke and Bridgwater [6] developed an analytical framework to describe the motion of particles through an array of solid surfaces such as may be encountered in spontaneous percolation or in the design of mixers or blenders having no moving parts. By means of numerical simulations they study the influence of the restitution coefficient, particle diameter and bar spacing on the performance of the disperser. They found that the characteristic jump length decreases with the size of the beads.

In a recent paper, Bruno et al. [7] have studied, both experimentally and numerically, a gravity-driven flow of disks through a hexagonal lattice of obstacles, a Galton board. During the fall, particles suffer dissipative collisions that scatter them in random directions: as a consequence particles trajectories are aleatory and a driven-diffusion regime is achieved. A characteristic length of the motion and the dependence with geometrical parameters of the system was analyzed in the steady regime for single particle and many particles flow experiments.

In the cited works, particles can percolate spontaneously by gravity in the medium, that is, they cannot be trapped by the geometry (the size of the percolating particles is sufficiently small compared to that of the packing particles). Inter-particle percolation can be induced too by applying a shear [8,9]. In all cases, the arrays of obstacles (or experimental media) were supposed to be large enough in order to avoid boundary or wall effects.

In this work we perform simulations of granular packings in 2-D by throwing disks into dies of varying width to represent the actual experiment of poured grains into a rectangular container until it is completely full. These simulated experiments will allow measuring percolation properties associated with the passage of small particles through the packings. The first aim of the present work is to find the dependence of those measured properties on the distance between the walls of the container where they are deposited. The second objective is to make a contribution to understand the dynamics of the process of mixing when percolation is present and that, otherwise, become difficult to measure in a real experiment.

In a previous paper [10], we have already reported an exhaustive characterization of similar arrays of disks as a function of their polydispersity. We found two important aspects. First, we established the dependence of a percolation parameter (critical shrinking factor b_c, defined further) on the radii dispersion (σ) of the packed disks. A power-law dependence was found. For small dispersion values, the system presents an abrupt crossover from non-percolative to percolative regimes. For greater values of

σ, the crossover smoothes. Second, relaxations produce a redistribution of stresses and displacements, lowering their strength.

In this scenario, which would be the role of the walls of the container in the dynamics of percolation? Does their effect depend on the value of σ?

In the following sections, we will present numerical results characterizing the percolative–non-percolative regimes for small particles diffusing through 2-D arrays of disks. We will show the effect of die walls on the crossover between those two regions. Moreover, we will get some conclusion on the way that the system will behave when mixing particles of different sizes.

2. Numerical aspects

In order to generate the packings, we employed the same computer algorithm already used in Ref. [10]. This algorithm has been programmed in a way that allows to generate packings of disks sampled from any desired size distribution. The time needed to set a packing of 10,000 disks and to obtain all the quantities of interest is just a few seconds, even on a Pentium III PC.

First, a radii distribution for the disks is selected and the desired number of disks that will form the pack, N_{total}, is selected. In the present simulations, disks radii were randomly chosen from a gaussian distribution with dispersion σ. First, the bottom of the packing is built by putting a number N of disks to ensure the desired wall separation. They are placed side by side.

After the bottom is filled, the remaining disks, $N_{total} - N$, are poured one at a time from the top of the die, at the middle point between the lateral walls of the container. Each grain falls down following a steepest descent algorithm: each new vertical position is updated by checking the maximum distance the disk can move down without overlapping an already deposited disk. At the first time it touches an already deposited disk, it rolls over it clockwise or counter clockwise, depending on the relative positions among the center of mass of the two touching disks. When the disk is rolling, we maintain a touching point over the surface of the already deposited disk and check for the presence of another disks in the way it is rolling through. If it finds a disk, we stop the rolling procedure and maintain the new point of contact with the second disk surface. Thus, the falling disk has two contacts: one with the first disk it touched as it was falling down vertically, and the other with the second disk it found as it was rolling. At this stage, we check whether a stable condition is fulfilled. We define a stable position when the center of mass of the disk falls in between the two points of contact of the disk with the other two already deposited grains. If it is the case, the grain is fixed in that position for the rest of the simulation run. If not, it will continue rolling, depending on the relative positions of its center of mass and the touching points. The rolling procedure goes on until another grain is touched and the stable position checking is performed again. This procedures is repeated until a stable configuration is attained by the particle.

Two different widths were used for the die. For each width, we run simulations for two extreme values of σ, i.e., 0.001 and 0.9. The scaling of the complete array of particles was conserved, i.e., the total number of particles poured into the die depended on the separation between walls in order to ensure the same number of layers in the system. This number of layers was of the order of 100, the same one used in Ref. [10]. In this way, we built up packings with $N_{total} = 800$ and 1500 disks, for bottoms containing $N = 8$ and 15 disks, respectively, and for both values of sigma.

3. Results and discussion

Suppose we have a packing of disks whose radii are randomly sampled from a gaussian distribution of mean R_m and dispersion σ, truncating its width to 4σ, i.e., the extreme possible values for the radii of the disks are $R_{max} = R_m + 2\sigma$ and $R_{min} = R_m - 2\sigma$. The small percolating particle has a radius R_p. To compare present results with the referred previous ones, we used the same values for $R_m = 2$ arbitrary units (a.u.) and $R_p = 0.2$ a.u. These values were kept fixed for the rest of our study.

Let us call L, the mean separation between lateral walls of the die, also measured in a.u. As explained above, we simulated four sets of arrays. Their parameters were, respectively, $\sigma = 0.9$, $L = 60$; $\sigma = 0.9$, $L = 32$; $\sigma = 0.01$, $L = 60$; $\sigma = 0.01$, $L = 32$.

For each set, a great number of equivalent samples was done to ensure that statistical deviations are small. Thus, statistical errors are smaller than any of the symbols used in all our plots.

Once the packing is generated, a shrinking process is started on disks radii to create empty space for the small particle to move through the array, i.e., each disk radius, R_i, is replaced by bR_i, where $b \in (0, 1)$ and is the same for all R_i, i.e., the shape of the radii distribution is unchanged. We call b_c to the critical value of b necessary for percolation through the die to occur.

After the shrinking process is performed, the small particle is launched from above. Assuming the die belongs to the XY plane, the little particle initial X position was ever fixed at $X = L/2$, and its initial Y position was at the top of the die. We did not allow random launching because, in that case, wall effects would be shadowed.

Because the size of the die affects the percolation threshold, we first looked for the possible shifts that previously calculated values of b_c could have. In Ref. [10] we determined that b_c was 0.7783 and 0.8992 for $\sigma = 0.9$ and 0.01, respectively. For the present values of L, we found that b_c was unaffected when $\sigma = 0.01$, whatever will be the value for L, and resulted to be equal 0.7690 and 0.6949 for $L = 60$ and 32, respectively. This means the diffusing particle has less number of ways to go through the packing when the walls are closer, making percolation harder.

Once b_c is determined, we studied the crossover from non-percolative to percolative regimes for the four sets of arrays.

In order to help the reader to understand the features of a typical packing of disks, we present four snapshots in Fig. 1 for both values of σ, and for the cases $b > b_c$ and $b < b_c$, as indicated. There, we show the system of disks as they are "seen" by the percolating particle, once the shrinking process has been performed.

We recorded the exit distributions for all the sets, i.e., exit frequency as a function of the transversal coordinate X_p. If particles are in the percolation regime, X_p is their

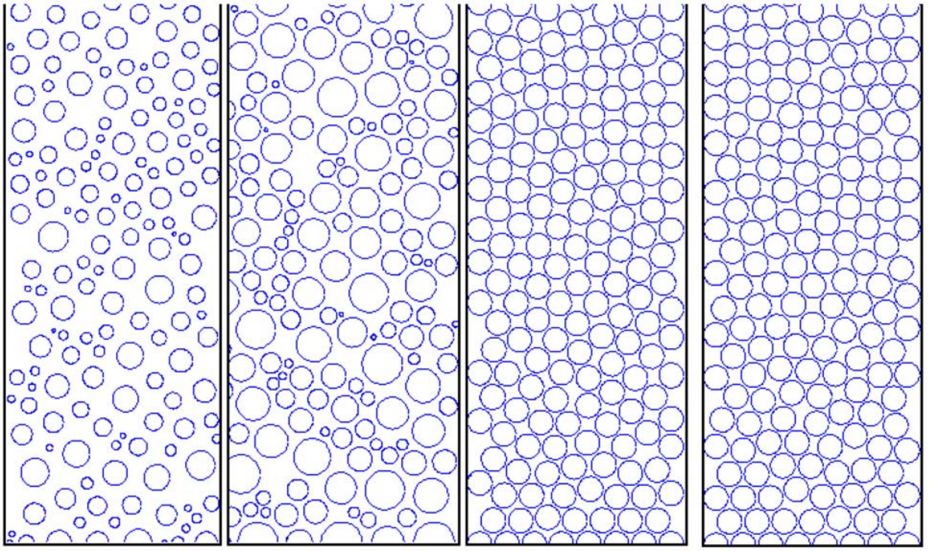

Fig. 1. Snapshots of part of typical packings of disks where little percolation particles go through. The values for dispersion and parameter b are respectively indicated.

final x-position at the exit. If particles are in the trapping regime X_p represents its final x-position, independently of their final y-position.

We repeated the measurements for several values of b close around b_c. Each distribution was then fitted with the theoretical function that resulted the best one for this purpose. The dispersion, Δ, corresponding to each fitting function was then plotted against b as depicted below.

Fig. 2 presents the results for $\sigma = 0.9$, parts (a), (b) and (c) corresponds to $L = 32$, 60 and, 400, respectively. They are all normalized in order to be compared and it is also important to explain the scale criteria used here for the transversal coordinate, X_p, in order to analyze the results correctly. The values for X_p in part (c) represent the coordinates of the particles in a container of 400 a.u., placing the container down left corner at the origin of the X-axis. In the plot, we just show the central part of the container, the one important for our measurements. For that reason, the center of the plot is at 200 a.u., coinciding with the center of the die. In part (b), we are still using the same "origin" of coordinates and place our die (with $L = 60$) with its down left corner at coordinate $X = 170$, in such a way that the center of this die coincides with the center of the die with width $L = 400$. The same criteria is used in part (a), but for $L = 32$, i.e., the down left corner of this die is at coordinate $X = 184$, in such a way that the center of this die coincides with the center of the other two dies.

As seen, part (c) shows the results for extremely separated walls, already obtained from Ref. [10]. Lines represent fitting functions. As clearly observed and indicated, there is a great amount of disks trapped at the walls for $L = 32$ and 60. This number

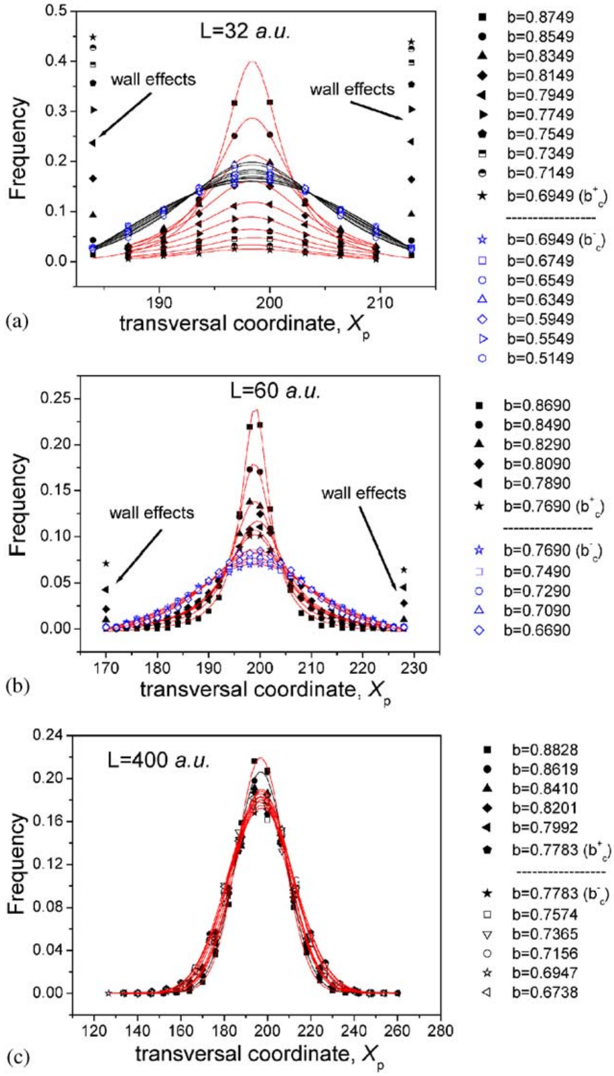

Fig. 2. Exit distribution functions for $\sigma = 0.9$, (a) for $L = 32$, (b) for $L = 60$ and (c) for $L = 400$. The corresponding b values for each histogram are indicated and the dot line serves as a guide to distinguish the percolating regime from the non percolating one. The minus and plus symbols over b_c indicate that the distribution corresponds to final X_p of trapped particles (b_c^+) and final exit X_p of percolating particles (b_c^-). Lines represent fitting functions.

increases as $b \to b_c$ because more and more disks get the chance of touching the walls. As b changes, qualitative behavior of distributions for different L is similar. As b decreases, the dispersion of distributions increases. We will discuss the details of this effect below. When fitting the distributions at the trapping region for $L = 32$ and

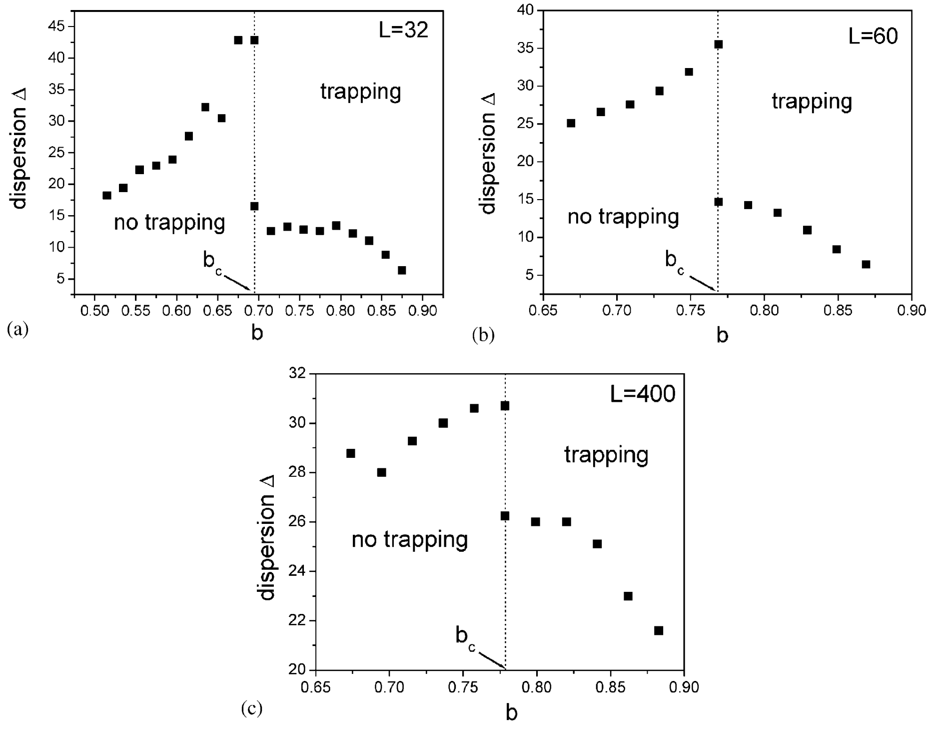

Fig. 3. (a-c) Crossover that suffers the width of exit distribution functions as b goes around b_c for $\sigma = 0.9$.

60, we observe that the proximity of walls breaks down the gaussian behavior. The shape of the distributions is closer to a lorenzian-like shape. We should mention here that fitting functions do not take into account the trapped particles at the walls.

For $b \leqslant b_c$, i.e., at the percolation region, lorenzian behavior is still present and this kind of function seems to be the best one fitting the "tails" of the exit distributions. This effect is still present for $b > b_c$, although gaussians also offer good fitting parameters. It is worthy to remember that, for the case of extremely separated walls, this effect was never present, i.e., exit distributions were always gaussians.

In Fig. 3 we show the dependence of the dispersion of the exit distributions on b. The crossover from trapping to non-trapping regimen can be appreciated. Like before, parts (a), (b) and (c) corresponds to $L = 32$, $L = 60$ and $L = 400$, respectively, part (c) being the results obtained in Ref. [10]. The crossover is steeper as the walls are closer. For lower separation, the gap for Δ is twice greater than for walls well apart. This feature is due to the reinsertion of particles from the walls, and becomes stronger as the walls get closer to each other. This effect is important when a mixture of particles of very different sizes is desired. In Fig. 4 and 5 we show the corresponding results for $\sigma = 0.01$. The results show some qualitative common aspect compared to the case $\sigma = 0.9$, but important distinctions should be highlighted. For both values of L, there is no entrapment of particles at the walls. The reason for this behavior is that

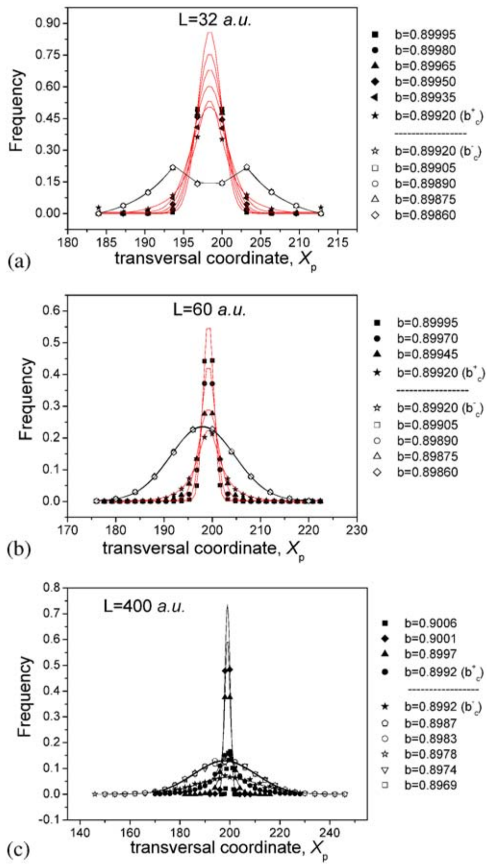

Fig. 4. Exit distribution functions for $\sigma = 0.01$, (a) for $L = 32$, (b) for $L = 60$ and (c) for $L = 400$. The corresponding b values for each histogram are indicated as they were in Fig. 1. Lines represent fitting functions. A can be seen, there are no trapped particles around the walls.

percolation likelihood for the particles is “step-like” for $\sigma = 0.01$, i.e., there exists a poor penetration when $b < b_c$ (abrupt increase of penetration depth around b_c, found in Ref. [10]). Thus, the particles do not get the chance to “see” the walls of the die. For that same reason, it was found that the shape of the exit distributions is gaussian-like as it was for extremely separated walls (Fig. 4, part (c)). We may say that, for poor polydispersity of the packing, wall effects become less important in the trapped region of penetration.

In the percolation region for $L = 60$, all fitting functions were gaussian in shape and they did not practically depend on b.

In the non-trapping region for $L = 32$ a curious behavior is observed. The exit distributions present a double peaked shape. This effect is caused by the feedback of particles returned by walls. Because of small polydispersity, arrays are quite ordered

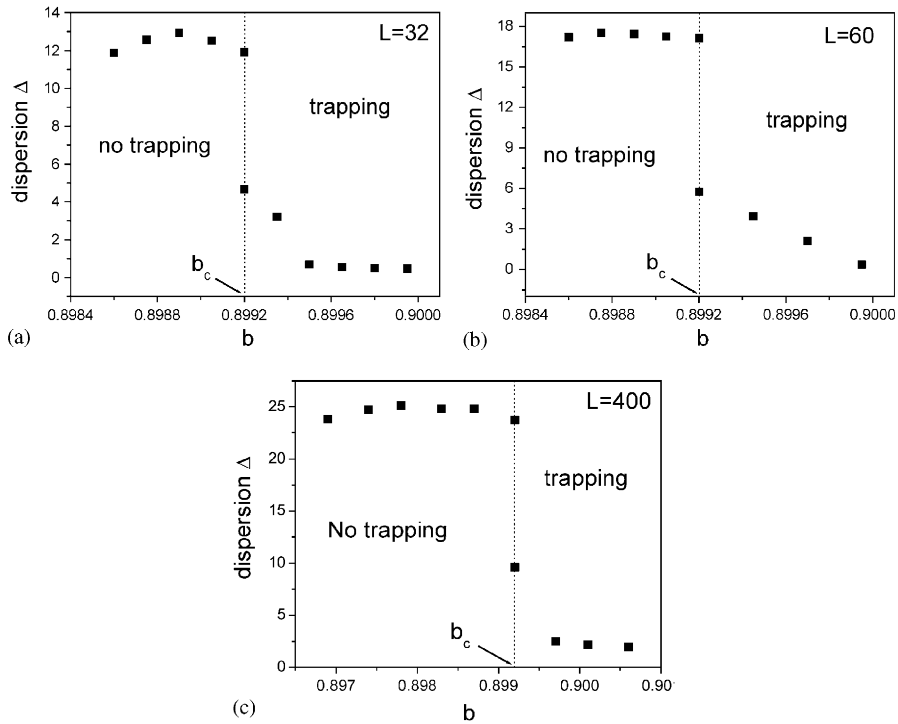

Fig. 5. (a-c) Crossover that suffers the width of exit distribution functions as b goes around b_c for $\sigma = 0.01$.

and there are diagonal ways back to the center of the packing and oriented in the same way. This effect was not observed for high polydispersity due to the disorder of the assembly of particles. This disorder allows a wider variety of ways back to the center of the array. Thus, the final exit x-position of the percolation particle could attain any value.

In Fig. 5 we show the crossover behavior for $\sigma = 0.01$ and different values of L. For the case of $L = 32$, Δ was considered as the width of the double peak fitting curve. Here the step in the crossover is practically independent of L. This feature is related to the fact that b_c does not change with the dimension of the die. This, of course, is due to the low polydispersity of the system.

Comparing the crossover behavior for different values of σ, we see that ordered packings present a practically constant dispersion Δ in the non-trapping region, while packings with greater polydispersivity, decrease the values of Δ as b is smaller. This is easily understood if one takes into account that, once percolation is possible for ordered packings, more open ways for the particle to diffuse do not produce any changes in their trajectories. On the other hand, in disordered systems, lower values of b create new ways for diffusion, dispersing the percolating particle.

4. Conclusions

In this paper we have studied the dependence on wall separation of percolation properties in two-dimensional arrays of disks. The present model does not take into account friction effects and it reports the pure steric response of packings to the diffusion of small particles. We found that, as the walls are closer, they produce a more pronounced crossover from non-percolation to percolation regimes. The reinsertion (feedback) of particles is the main cause of this effect and it is stronger for high values of polydispersity.

The proximity of walls changes the shape of the exit distribution functions of small particles, both in trapping and non-trapping conditions. The shape of these functions seems to be lorenzian-like in stead of the classical gaussian-like behavior found earlier.

Particles get trapped at the walls when polydispersity σ is high due to the fact that they can percolate easier and their likelihood to touch lateral walls is higher than for low values of σ.

Finally, ordered packings (low σ) present double-peak exit distributions in the percolation regime. This feature is due to the periodic-like configuration that these packings have, i.e., particles get back to the center of the packing once they touch the walls almost in the same way (lack of disorder) contributing to the formation of those peaks in the exit distributions. Further efforts still are needed to better characterize the passage of small particles through two-dimensional packings. The addition of friction and bouncing are the next steps to explore in our present model of percolation.

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