LETTER TO THE EDITOR

First-order phase transition in piling problems

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Abstract. We consider the geometrical properties of the 'skeleton' which supports mechanically the structure of a piling of discs with fluctuating radii in two dimensions. We show that this skeleton is part of a sublattice which can be obtained from a geometrical filtering procedure. In the case of a randomly diluted lattice, this geometrical construction defines a generalisation of a 'bootstrap percolation'. We show by a numerical simulation of this problem that it leads to a first-order phase transition, for an initial fraction of present bond close to 0.84. Some implications for the properties of the skeleton are discussed.

The geometrical structure of disordered packings is very dependent on the physical constraints imposed during its building procedure or algorithm. If one is interested in the grain space (the complementary part in a packing is the porous space), one of the most important features of this geometrical structure is that it presents a disorder of contacts [1]: there exist many pairs of neighbouring grains which are separated by a small distance. A slight change in the geometry of the packing is likely to bring these particles into contact. In order to illustrate this, we first consider the case of an ordered packing of regular equal discs. We can map this packing onto a lattice by assigning a site to each disc centre and by connecting the sites with a bond whenever the two discs are in contact. In this case, the lattice is an ordered triangular one. But if the discs are no longer perfect, for example if their radii are fluctuating at random, the corresponding lattice is 'diluted' since some contact between neighbouring particles will be broken.

A first step in the modelling of such a problem is to use a construction introduced in this connection by Dodds [2]: starting from a completely triangulated lattice, it consists in randomly cutting some bonds in order to ensure the required mean coordination number $\langle z \rangle$ of the packing. This construction is useful in understanding the connection between percolation and granular media [3], but it is somewhat artificial since local stability criteria (stability under gravity, for example) impose a minimum number of contacts between each disc and its neighbours and some additional geometrical constraints on their relative orientations. Therefore, the random dilution is a first crude approximation. The precise structure of the packing in reality is very sensitive to the physical process which will govern the local restructuring of the packing [4], or the type of algorithm used to model it [5]. The final value of $\langle z \rangle$ is 4 for disordered two-dimensional
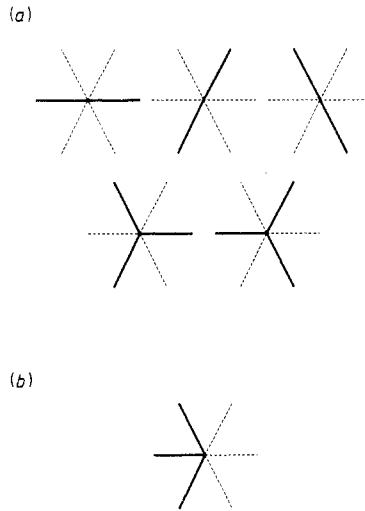
(a)

(b)

Figure 1. (a) The five basic allowed configurations of bonds around a site which can sustain compressive forces are shown. Any superposition of these five configurations is also allowed. (b) One example of a forbidden configuration, since the requirement that all forces are compressive implies that these three bonds are stress free.

packings of discs built grain after grain under gravity (without any further reorganisation), but it can be different if collective equilibrium is allowed [6], or if another stability criterion (instead of gravity) is imposed [7]. The geometry of the system is not solely defined by a local criteria, but is also dependent on more global conditions. For example, if it is submitted to an external pressure applied at its perimeter, the whole system must generate a rigid 'skeleton' (very comparable to that described in this Letter) able to resist pressure, as can be seen by photoelastic observations [8]: the term skeleton is suitable because a large part of the contacts between grains does not carry any stress, and only a tenuous subset is responsible for the elastic properties of the medium. So, from this point of view, the representative lattice of the packing and the skeleton supporting the stress is the result of the application of both local and global constraints.

As a limit of this model, we first consider a dilute lattice in which $(1-p)$ bonds have been randomly removed, as in the Dodds model; p, the fraction of bonds present, is a free parameter, which in some way measures the amount of disorder. Now, in this diluted triangular lattice, we want to model the elastic skeleton by taking into account the fact that each contact in the packing, or each bond in the lattice, is allowed to carry a compressive force, but not a tensile one (cohesionless packings). This constraint imposes some geometrical limitations: in particular, in figure 1(a), we show the basic configurations of bonds at one site which are acceptable using this criterion. All those configurations, and superposition of them are acceptable, whereas all others (such as the one shown in figure 1(b)) violate the requirement of elastic equilibrium and positivity of each force at the same time.

To study the effect of this constraint on the random dilution process, we have constructed random triangular lattices, with a given initial concentration of bonds present p. On those lattices, we have 'filtered' out the bonds that could not support any stress according to the above-mentioned criterion. This procedure has been repeated for various lattice sizes ranging from 20×20 to 100×100, and with up to 100 lattices for the most important values of p (see below) (0.80 to 0.90). The boundary conditions used are such that the packing is considered to be inside a box, and therefore, the sites lying on the border of the lattice are not 'filtered'. The shape of the lattice we considered
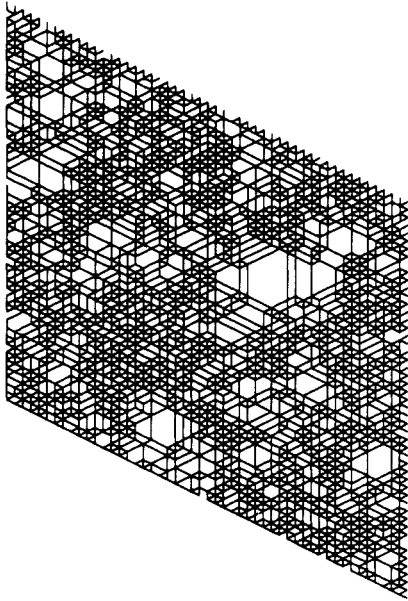
Figure 2. An example of a 50×50 lattice, initially diluted with $p = 0.85$, after the filtering procedure. Although the structure seems to be very dense, the removal of a very small fraction of the bonds (less than one per cent) would result in the complete destruction of the lattice through the filtering procedure.

was chosen to be diamond, for simplicity, although neither the shape of the lattice nor the boundary conditions used are likely to change the result we report below. Figure 2 shows an example of such a lattice of size 50 once the filtering procedure has reached a final invariant configuration.

The algorithm we used to filter out the lattice is the following. We use a bit-coding of the configuration of present or absent bonds around each site. A site is given a number, z (between 0 and 63), whose binary expression is a series of six digits 0 or 1, each of them telling if a bond with a given orientation is present (1) or absent (0). The allowed configurations shown in figure 1(a) are thus coded by the numbers $a_1 = 9$, $a_2 = 18$ and $a_3 = 36$ for the three two-bond configurations, and $a_4 = 21$ and $a_5 = 42$ for the two three-bond ones. The filtering of a given site configuration, z, is z' given by the union of all the basic configurations which are contained in the local configuration:

$$z' = \mathrm{OR}_i(a_i) \tag{1}$$

for i such that

$$(a_i \ \mathrm{AND} \ z) = a_i \tag{2}$$

where OR and AND refer to the bit-wise Boolean operations. Finally, the numbering of neighbouring sites configurations was updated consistently with the filtering.

For each lattice, we have recorded the final concentration of bonds, $q(p)$. Figure 3 shows the typical results of $q(p)$ where each point corresponds to one lattice of size 100. Surprisingly, we see that these points form two very distinct subsets, one for low values of q and one for large. The non-zero value of low q is an artefact of the simulation. As mentioned above, the sites at the border on the box are not filtered. Then the low value of q corresponds to the remaining sites attached to the border of the lattice. Obviously it vanishes at the thermodynamic limit (i.e. for an infinite lattice).

More importantly, it appears that it is not possible to generate a randomly diluted lattice such that the final concentration of bonds lies in an intermediate range. This fact
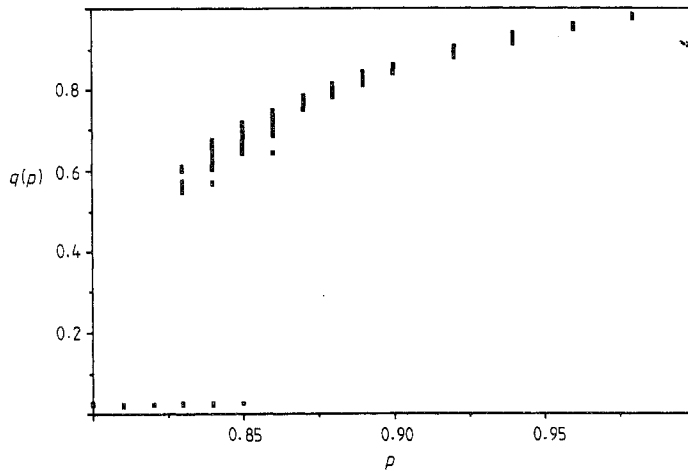
Figure 3. The fraction of bonds present, $q(p)$, after the filtering procedure, as a function of the initial bond concentration, p. Each point corresponds to one lattice of size 100×100. The discontinuity of the curve reveals that the transition is first order.

reveals that the transition we observe is discontinuous or *first order* in the language of phase transition.

Asymptotically, there exists a well defined threshold p_c, which separates the two ranges of values of q. From our numerical simulations we estimate this threshold to be

$$p_c = 0.84 \pm 0.01. \tag{3}$$

Because of finite size effects, there is some overlap between the minimum value of p for which q will be large, and the maximum value of p for which q will be small. However, we note that this overlap in p-values decreases as the lattice size increases.

In fact, this process is very much reminiscent of 'bootstrap percolation' [9, 10]. In this statistical model, for a dilute lattice, one filters the bonds in such a way that each site has a minimum of m neighbours, where m is a free parameter. Finally, one records the mass of the largest cluster as an order parameter. One could also record the density, r, i.e. this mass divided by the lattice size. For $m = 1$, this filtering process is useless (the filtered state is identical to the initial one) and therefore the only important fact is the selection of the largest cluster; this is exactly a percolation problem. In that case, r is known to go to zero at a threshold value of p, the percolation threshold, p_c, following the *continuous* evolution:

$$r \propto (p - p_c)^\beta \tag{4}$$

where β is a critical exponent. In this sense, percolation is a second-order phase transition. For instance, in two dimensions, $\beta = \frac{5}{36}$ [11].

For $m = 2$, all tree-like structures are removed. For a space dimension less than six, loops are relevant in a percolation problem, and therefore the number of bonds removed by the filtering procedure is negligible compared with of the number of bonds which are not counted because they do not belong to the largest cluster. Therefore, once more, one encounters a percolation-type behaviour, with the same critical exponent as for the $m = 1$ case. Above six dimensions, loops are no longer relevant and therefore the filtering process will remove a large part of the infinite cluster above at the percolation

threshold. Indeed the analytic solution on a Bethe lattice (which mimics a space dimension above six) shows that the transition is still second order but with a different critical exponent ($\beta = 2$ instead of $\frac{1}{2}$).

For values of m larger than two, on a Bethe lattice, it can be shown [9] that the transition becomes first order. For space dimension less than six, the situation is more complex, and is still being studied (see [10]).

In the case we have studied, the parallel with a bootstrap percolation process is clear. The only difference is that the filtering rules makes use of the orientation of the bonds and not only of their number. Thus it appears natural to find a first-order phase transition. We also note that, in our case, there is no need to remove the isolated finite clusters, since they are automatically removed by the filtering procedure. This is physically sound, since there cannot be any stress transmitted through an isolated cluster, nor is it possible to find any self-equilibrated pre-stress configuration where all forces are compressive.

What consequences can we derive from this result for real packings, and for the elastic skeleton of these pilings? Two points should be addressed: first, the relevance of the dilution of the lattice introduced at the initial state of the lattice, and second, the filtering procedure.

For the first point, as discussed in the introduction, a limitation comes from the fact that local stability generally imposes a minimum number of contacts for each grain (usually two in two dimensions), in contrast to a random dilution. But except for some specific piling (low coordination number or some specific binary distribution of radii), the induced geometrical differences between real packings and the Dodds model (i.e. random dilution model) are small. On the other hand, it should be noted that in real packings, fluctuations of the radii of the elements that are piled up will introduce some correlations in the representative lattice. These correlations can be important (long range) since the perturbation introduced by a defect is transmitted to its neighbours in an additive fashion. (Notice that the fact that the piling must remain a slight perturbation of an ordered one, and thus that the maximum fluctuations should be small compared to the mean radius is an additional constraint which should not be confused with the previous one).

These correlations have been studied in a particular case, where the rules used to build the packing render the problem simple [12], but they can be forgotten in the limiting case where the radii fluctuation is very singular at zero [13]. At last, for disordered piling (for example in the case of relatively large distribution of radii), they are only short range [14]. In fact, because our filtering procedure uses essentially the orientation of the bonds as underlined above, the most important correlations are orientational. Note that the importance of that orientational order has been stressed too in the case of the mechanical properties of two-dimensional packings of cylinders [15]: the above-defined skeleton, observed by photoelasticity, is very sensitive to this order, and the macroscopic stress–strain characteristic too. If these different correlations are likely to modify the numerical value of the threshold, however, the order of the transition is most probably unchanged.

Let us accept the dilution process as a first approximation, and discuss the relevance of the filtering construction. Obviously, the elastic skeleton of a given piling must be stable with respect to the filtering procedure. This implies that it should be part of the filtered lattice, without necessarily being identical to it. In consequence, we expect a change of behaviour for a well defined concentration of present bonds, p^*, larger than the threshold obtained here, since there does not exist any solution for p below it. The physical meaning is that below p^*, the piling is not stable; so, some large geometrical

deformations and restructuring have to take place so as to find another stable skeleton, starting from a less-diluted lattice.

A direct investigation of the structure of the skeleton of a three-dimensional random packing is currently being studied experimentally [16], and numerically in two dimensions [17]. The structure of this skeleton is determined both by the solution of the force distribution inside the lattice according to the usual elasticity equations, and the additional constraint that all forces should be positive. This renders the problem much more difficult than the approach developed here, since it is non-local in much the same way as the central-force elasticity problem is. On the contrary, the filtering procedure developed here is purely *local*. This simplification implies that we only get a bond on the admissible skeleton. However a preliminary study [17] indicates that the first-order character of the transition is preserved in the complete problem.

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