The hierarchical properties of contact networks in granular packings

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The topological structure resulting from the network of contacts between grains (contact network) is studied for very large samples of disorderly-packed monosized spheres with densities ranging from 0.58 to 0.64. The hierarchical organization of such a structure is studied by means of a topological map which starts from a given sphere and moves outwards in concentric shells through the contact network. We find that the topological density of disordered sphere packing is larger than the topological density of equivalent lattice sphere packings.

1 INTRODUCTION

To identify the accessible configurations at the grain level and to understand which are the possible combinations of such local configurations which generate the global packing is of singular importance, hence it is the necessary starting point for any fundamental understanding of granular matter. Until now the empirical investigation of the geometrical structure of granular packings have been limited by the paucity of accurate experimental data. Indeed, after the seminal works of Bernal, Mason and Scott (Bernal & Mason 1960, Scott 1962), it has been only very recently that the use of tomography has allowed one to ‘see’ the three dimensional structure of such systems and explore their geometry from the grain level up to the whole packing (Seidler et al. 2000, Sederman et al. 2001, Richard et al. 2003, Aste et al. 2004, Aste et al. 2005).

In this paper we report and discuss results from an empirical investigation by means of X-ray Computed Tomography on very large samples of disorderly packed monosized spheres with densities\(^1\) ranging from 0.58 to 0.64. This study is the largest and the most accurate empirical analysis of disordered packings at the grain-scale ever performed. A detailed description of the experimental methodology and apparatus are reported in (Aste et al. 2004, Aste et al. 2005). We analyzed 6 samples of monosized acrylic spheres in cylindrical containers with roughened walls, and with an inner diameter of 55 mm, filled to a height of \(\sim 75 \text{ mm}\). In order to verify possible effects due to gravity and sizes we used two kind of acrylic spheres with diameters \(d = 1.00 \text{ mm}\) and and \(d = 1.59 \text{ mm}\), with polydispersities within 0.05 mm. The

\(^{1}\)The density is defined as the fraction of the volume occupied by the balls divided by the total volume of the region of the space considered.
smaller spheres were used to prepare two samples (referred as sample A and C hereafter) at densities 0.586 and 0.619 containing about 103,000 and 143,000 spheres, respectively. Whereas, the larger spheres were used to prepare four samples at densities 0.596, 0.626 0.630 and 0.64 (samples B, D, E and F) each containing about 35,000 beads. A X-ray Computed Tomography apparatus (see Sakellariou et al. (Sakellariou et al. 2004)) was used to image the samples. The two large samples (A, C) were analysed by acquiring data sets of $2000^3$ voxels with a spatial resolution 0.03 mm; whereas for the other four samples (B, D, E and F) were acquired data sets of $1000^3$ voxels with a spatial resolution 0.06 mm. The positions of the center for each sphere were retrieved, with a sub-voxel precision, by a convolution method applied to the segmented (Sheppard et al. 2004) datasets (see (Aste et al. 2004; Aste et al. 2005) for further details).

2 Coordination Number

The average number of spheres in contact with any given sphere have been widely investigated in the literature of granular matter (Bernal & Mason 1960, Scott 1962, Seidler et al. 2000; Aste & Weaire 2000, Saderman et al. 2001; Silbert et al. 2002; Donev et al. 2004). Indeed, this is a very simple topological quantity which gives important information about the local configurations and the packing stability and determines the cohesion of the material. The average number of spheres within a radial distance $r$ from a given sphere ($n_t(r)$) increases with the radial distance. Its empirical behavior is shown in Fig[2] One can note that above $r = 0.98d$ the number of neighbors grows very steeply up to a ‘knee’ at about 1.02d where a slower growth takes place. The definition of the coordination number depends therefore on the radial distance within which two spheres are considered in contact. However, a deconvolution method developed in (Aste et al. 2005) can be used to distinguish between the contribution from the spheres in contact and the contribution from other spheres which are near but do not touch. We estimate that in the 6 samples A-F the average number of spheres in contact $n_c$ are between 5.81 and 6.97. In fig[1] the values of $n_c$ are reported as a function of the sample densities showing a clear and consistent increasing trend with the density. Such dependence on the packing density (Fig[1]) has important conceptual implications which are discussed in (Aste et al. 2005).

In this paper we construct ‘contact’ networks by using different thresholds on the distance within which two spheres are considered in contact. This produces several different contact networks with average coordinations ($n$) that increase with the threshold distance.
3 Topological Structure Beyond First Neighbors

Any force-path or any infinitesimal local grain displacement must mechanically propagate from grain to grain through the network of touching grains. The understanding of the hierarchical organization of such contact network beyond first neighbors is therefore crucial. Here we apply to granular matter an approach which was originally developed for the study of crystalline systems (Brunner & Laves 1971; O’Keeffe 1991b; Conway & Sloane 1997; Grosse-Kunstleve et al. 1996). Following the definition of O’Keeffe (O’Keeffe 1991a), for these crystalline systems, the asymptotic behavior of $K_j$ can be characterized in terms of an ‘exact topological density’: $TD = \langle a_j \rangle / 3$ (Grosse-Kunstleve et al. 1996). It has been noted that such a topological density is interestingly related to the geometrical density of the corresponding crystalline structure and it is a powerful instrument to characterize such systems. For instance, it is easy to compute that the cubic lattice has $K_j = 4j^2 + 2$. Whereas, spheres packed in a bcc (body centered cubic) crystalline arrangement have: $K_j = 6j^2 + 2$ $(j > 0)$. On the other hand, it has been shown (Conway & Sloane 1997) that for Barlow packings of spheres, $K_j$ are always in a narrow range within:

$$10j^2 + 2 \leq K_j \leq \left\lfloor \frac{21j^2}{2} \right\rfloor + 2 \quad (j > 0), \quad (1)$$

where the brackets $[...]$ indicate the floor function. It has been observed by O’Keeffe and Hyde (O’Keeffe & Hyde 1996) that for lattice sphere packings with coordination number $n$, the general rule holds: $K_j = (n-2)j^2 + 2$, implying therefore $a = n - 2$.

Beyond perfect crystalline order very few results are known either from theoretical, empirical or numerical point of view. One can argue that $K_j$ must grow with a law comparable with the law for a spherical shell: $K_j \sim aj^2 \sim 4\pi j^2$. However, it is also clear that the shape of the growing shell and its roughness can drastically change the coefficient $a$ (as observed in two dimensional cases (Aste et al. 1996)).
Figure 3. Shell occupation numbers vs. topological distance. The symbols indicate the different samples (as in Fig.1) and the lines are the best-fits (of the growing part only) using the polynomial form: \( K_j = a j^2 + c_1 j + c_0 \). The fits are between \( j = 2 \) and \( \hat{j} = 10 \) (for samples B, D, E, F) and \( \hat{j} = 15 \) (for samples A, C). The data refer to threshold distance 1.05d.

Moreover, it can be shown (Aste et al. 2005) that in some topological networks the law of growth can follow an intrinsic dimension which is different from the dimension of the embedding space (3 in our case). This mechanism can produce power law growth with exponents different from 2, or different behaviors such as exponential – or even faster – laws of growth (Aste et al. 2005).

We observed that the number of spheres at a given topological distance \( j \) from a central one follows a power law growth (see Fig.3) until a critical distance \( \hat{j} \), above which the shells hit the sample boundaries and \( K_j \) starts to decrease. We verify that a quadratic law \( K_j = a j^2 + c_1 j + c_0 \) fits quite accurately the observed behaviors of \( K_j \) for \( j < \hat{j} \). This fixes the intrinsic dimension for these systems equal to 3 (which coincides with the geometrical dimension of the embedding space).

We find that the coefficient \( a \) depends on the threshold distance within which neighboring spheres are considered in contact. Indeed, changes in the threshold distances are unavoidably associated with changes in the contact network and an enlargement of the threshold distance must correspond to a thickening of the shell. It has been noted previously that such a threshold affects also the average coordination number \( n \) in the contact network (Fig.2). In Fig.4 we show that these two quantities are positively correlated: the coefficient \( a \) increases monotonically with \( n \). Interestingly, a comparison with the known behavior in lattice sphere packings (\( a = n - 2 \)) shows that these disordered systems are topologically more compact than the analogous lattices. This observation might be relevant when the structural stability and rigidity of such systems are concerned. Understanding whether this is a bare consequence of topological disorder or it is associated to the properties of such granular systems is a challenging topic which must be explored.

4 CONCLUSION

The study of the topological structure of the contact network at the grain level shows that the average number of spheres in contact in-
creases almost linearly with packing density and lies between 5.5 and 7.5 in the range of densities between 0.58 and 0.64. An extrapolation to the random loose packing density \( \rho = 0.55 \) suggests that at this density the system could have an average number of 4 neighbors per sphere. This implies the possibility of a rigidity percolation transition taking place at the random loose packing limit.

The structure beyond first neighbors, studied by means of a topological map, shows that the contact network has an intrinsic dimension of 3. Surprisingly, we found that the topological density in disordered sphere packings is always larger than the topological density in the corresponding lattice sphere packings. Such a larger topological density is an indication that the contact network is more compact in disordered systems despite the fact that the geometrical density is lower. This fact might have important implication on the system stability and resilience to perturbations and shocks. Notably, this fact is consistent with what we observed in (Aste et al. 2005) where we found that in a certain region around the grains, disordered packings can be locally more compact than the crystalline ones.

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