

On universal structural characteristics of granular packs

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Understanding the dependence of the structure of granular materials on grain parameters is key to predictive modelling of granular matter. Structural characteristics are commonly believed to be sensitive, for a given packing process, to intergranular friction, particle size distribution and initial conditions. We show here that the intergranular friction coefficient and the initial conditions are details, which can be scaled away, and that structures are determined mainly by the packing dynamics and the grain size distribution. This we do using the quadron description to analyse the structures of a number of numerically-generated planar disc packs in mechanical equilibrium, varying all these parameters. Our findings are as follows. 1. The mean coordination number is a universal function of the packing fraction, independent of the initial conditions, intergranular friction and size distribution we used, when "rattlers" are ignored. 2. For a given packing process and disc size distribution, both the total and conditional quadron volume distributions collapse to universal forms, independent of the initial conditions and intergranular friction. 3. The cell order distribution collapses to a universal form for all friction coefficients, initial conditions and for the two disc size distributions we studied. These results suggest that mechanically stable granular structures are determined mainly by the packing dynamics and the grains size / shape distributions - the effects of the intergranular friction and initial state can be scaled away and are therefore predictable.

Characterization of the structure of solid random granular systems is of primary importance in science and engineering [1–6]. A central quest in the field is for relations between the physical properties of mechanically stable many-grain packs and their structural characteristics. Yet, there are many such characteristics and there is no systematic way quantify such relations. Moreover, different structural properties often correlate well with different physical properties. For example, void size distribution and connectivity correlate well with permeability to flow, which is relevant to underground water, pollutant dispersion and oil extraction [2]; catalysis and heat exchange between the grains and a fluid in the void space are more sensitive to the solid-void surface distribution [3]; and the mechanics of granular solids is governed by an interplay between the structure and the force transmission through the intergranular contacts [4]. The problem is complicated by the many observations that the structural characteristics depend on the distributions of grain shapes, sizes, intergranular friction coefficients and preparation history. Consequently, there is no understanding of any "universal" structural characteristics, i.e. which are independent of some of these parameters.

The aim of this paper is to identify such universality and to show that, contrary to current belief, the distributions of a number of structural features of random packs of planar (2D) granular solids collapse to common forms for all intergranular friction coefficients and a range of initial preparation states.

We analyse the structure of numerically generated and mechanically equilibrated 2D polydisperse disc packs, using the quadron-based structural description[4, 7, 8]. In

this method, illustrated in Fig. 1, one first defines the centroids of grains (discs) g and cells c as the mean position vectors of the contact points around them, respectively. Next, the contact points around every disc are connected to make polygons, whose edges are vectors, \vec{r}^{gc} , that circulate the grain in the clockwise direction. Then, one extends vectors \vec{R}^{gc} from the disc centroids g to the cell centroids c that surround them. A quadron is the quadrilateral whose diagonals are the vectors \vec{r}^{gc} and \vec{R}^{gc} . In the absence of body forces, equilibrated cells are convex and, for convex grains, the pairs \vec{r}^{gc} and \vec{R}^{gc} generically intersect. For brevity, we index the vectors defining a quadron by q rather than gc . The quadron's shape is quantified by the structure tensor $C^q = \vec{r}^q \otimes \vec{R}^q$ and its volume is $V_q = \frac{1}{2} | \vec{r}^q \times \vec{R}^q |$ providing a quantitative measure of the local structure.

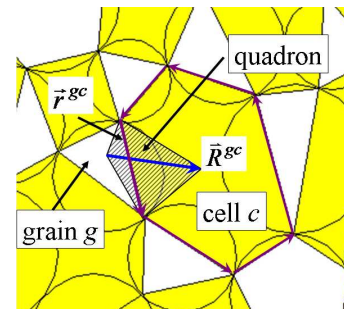


FIG. 1. The quadron (shaded) is the quadrilateral whose diagonals are vectors \vec{R}^{gc} and \vec{r}^{gc} , defined in the text.

This description is convenient for measuring local structural characteristics and, as such, has a significant advan-

tage over methods that average over arbitrarily-defined structural properties. The tessellation by quadrons is also preferable to Voronoi-based tessellations[2, 3, 6, 9] both because it makes possible an unambiguous local tensorial description and because it preserves the connectivity information.

For our numerical experiments we used the Discrete Element Method (DEM)[10, 11], in which disc motions follow Newton's second law with an incremental time marching scheme. For the interaction between discs, we use a repelling harmonic interaction potential, characterised by normal and tangential spring constants, k_n and k_s , respectively, activated on contact and overlap between discs. Without loss of generality, we set $k_s/k_n = 1/4$ in this study.

Aiming to study polydisperse systems, we chose two disc size distributions (DSDs). One is log-normal, due to its wide use in civil engineering and soil sciences[12], $P(D) = \exp[(\ln D - \ln D_0)^2 / 2\sigma^2] / \sqrt{2\pi}\sigma D$, with $D_0 = 1.0$ and $\sigma = 0.2$, whose mean disc size and mode are, respectively, $\bar{D} = 1.02$ and $D_{mode} = 0.961$. The other is uniform, $0.663 \leq D \leq 1.38$, having the same average and dispersion.

Our granular systems are generated as follows. First, we construct three random packs in a double periodic domain, engineered to be on the verge of jamming. The packs consist of 21400 ± 1000 discs and are made at packing fractions $\phi = 0.76, 0.82$ and 0.84 for the log-normal DSD systems and $\phi = 0.76$ and 0.84 for the uniform DSD systems. The small variation in the numbers of particles is due to the different densities of these initial configurations. These loose-, intermediate- and dense configurations are used as initial states (respectively, LIS, IIS and DIS) for a subsequent packing procedure as follows. All the discs are assigned a friction coefficient μ and the system is subjected to a slow isotropic stress σ_c by changing the periodic length in both directions. We limit the applied stress such that the average overlap discs is $\delta = \sigma_c/k_n = 10^{-5}$. No gravitational force is used and the compression continues until the fluctuations of disc positions (per mean disc diameter) and intergranular forces (per mean average contact force) are below very small thresholds - 10^{-9} and 10^{-6} , respectively. This procedure is carried out from each initial state for five different values of μ : 0.01, 0.1, 0.2, 0.5 and 10, giving altogether 15 different systems of log-normal DSD and 10 systems of uniform DSD.

For every system, we computed the packing fraction, the mean coordination number, and a range of structural properties to be described below. For the determination of \bar{z} , we disregarded 'rattlers', i.e. discs with one or no force-carrying contact. The dependences of \bar{z} on ϕ are shown in Fig. 2. The upper and lower bounds, $\bar{z}_{max} = 4$ and $\bar{z}_{min} = 3$, correspond generically to isostatic states of smooth ($\mu = 0$) and frictional ($\mu \rightarrow \infty$) discs, respectively. The three systems with $\mu = 0.01$ settle into states

that are very close to the ideal frictionless jammed state: $(\bar{z}, \phi) = (3.941, 0.840), (3.944, 0.842)$ and $(3.943, 0.843)$, respectively. However, as μ increases there appear differences between the (\bar{z}, ϕ) -points of the final states, as shown in Fig. 2.

To study the mean quadron volumes, it is convenient to normalize them by the mean disc volume after removing rattlers \bar{V}'_g , $v \equiv V_q/\bar{V}'_g$. In Fig. 3, we plot v against \bar{z} for all the systems and discover that all the points fall nicely on one curve.

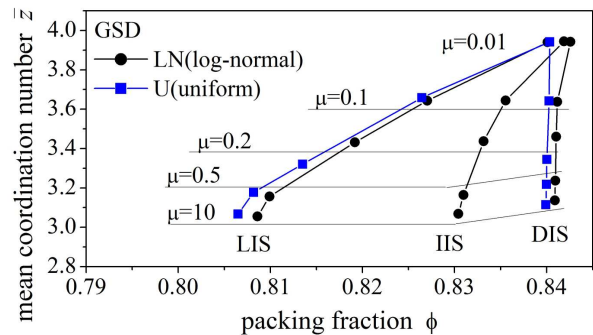


FIG. 2. Mean coordination numbers vs. packing fractions for all our systems. Different initial states (LIS, IIS, DIS) and disc friction coefficients ($\mu=0.01, 0.1, 0.2, 0.5, 10$) give distinctly different final jammed packs.

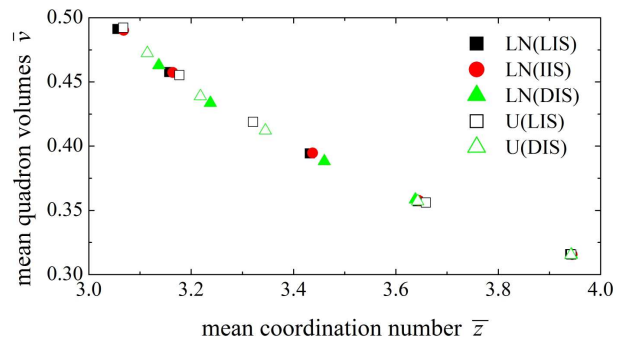


FIG. 3. The mean quadron volume \bar{v} vs. the mean coordination number \bar{z} . The graph collapses for all intergranular frictions, all initial states and both DSDs.

As we shall see further below, key to understanding this collapse is the discarding of the rattlers. The rattler-free packing fraction is

$$\phi' = \frac{V'_s}{V} = \frac{\sum^{N'_g} V_g}{\sum^{N_q} V_q} = \frac{N'_g \bar{V}'_g}{N_q \bar{V}_q} = \frac{1}{\bar{v}\bar{z}} \quad (1)$$

where V is the total volume, V_s is the solid volume, V_g is the volume of disc g , \bar{V}'_g is the discs mean volume, N_g is the total number of discs, the primed variables correspond to the rattler-free system. Based on (1) and

the collapse in Fig. 3, we expect ϕ' to be a function of \bar{z} alone, which is confirmed in Fig. 4. Note that this collapse is in contrast to current wisdom [6, 13].

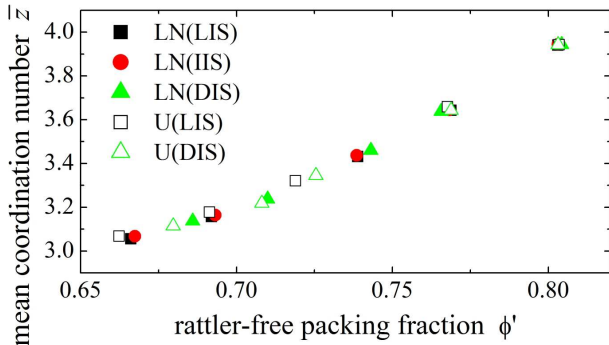


FIG. 4. The collapse of the relation between mean coordination number and rattlers-free packing fraction.

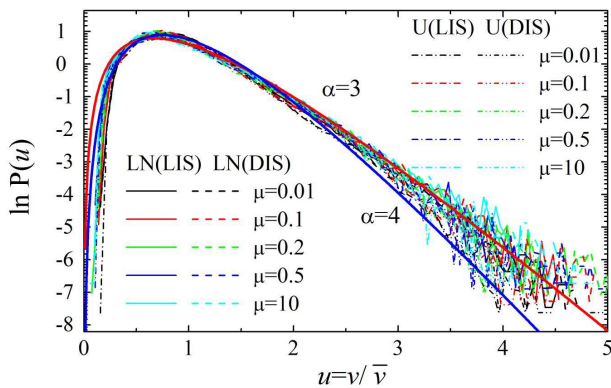


FIG. 5. The collapse of the PDFs of the normalized quadron volumes, $u \equiv v/\bar{v}$, for all the systems, compared with two Γ distributions (Eq.(2)), with $\alpha = 3$ and 4.

As seen from Figs. 4 and 2, the rattler-free packing fractions are considerably smaller, but it is the latter packing fractions that are commonly reported in the literature. Significantly, the collapse of the plots in Fig. 2 shows that the differences for different initial state is only due to the different rattler fractions. It is also interesting to note that, while the curves of Fig. 2 are sub-linear, their collapsed rattler-free form is super-linear. This collapse prompted us to consider more closely the probability density functions (PDFs) of the quadron volumes. Since the mean quadron volume increases with μ , we scale the quadron volumes by their means, $u \equiv V_q/\bar{V}_q = v/\bar{v}$. We find that this is sufficient to collapse the PDFs of all the systems almost perfectly onto one curve *independent of both friction and initial state* (Fig. 5).

The collapsed PDF appears to have an exponential tail, lending support to the granular statistical mechanics formalism[1], as this may be the signature of the Boltzmann-like factor. Our best fit to the collapsed curve is the Γ distribution

$$P(u) = \frac{\alpha^\alpha}{\Gamma(\alpha)} u^{\alpha-1} e^{-\alpha u} \quad (2)$$

with α between 3 and 4. These observations have several implications. (i) The quadron description makes possible to collapse the statistics of all the systems, thus providing better insight into the fundamental characteristics of granular packs. (ii) The structural characteristics are determined by physical mechanisms that transcend the effects of friction and initial states, which can be scaled away. (iii) The collapse is only possible when disregarding rattlers, which do not transmit forces, suggesting an inherent relation between the structural characteristics and the self-organisation of the force-carrying backbone during the packing process.

To explore the origin of the above collapses, we use a recently-proposed decomposition of the quadron volumes into conditional PDFs[14]

$$P(v) = \sum_e e Q(e) P(v|e) \quad (3)$$

where $Q(e)$ is the occurrence probability of cells of order e and $P(v|e)$ is the conditional PDF of the normalized quadron volume, given that it belongs to a cell of order e . Frenkel et al.[14] argued, on the basis of geometrical considerations, that $P(v|e)$ should be independent of intergranular friction. Their argument was that, given a collection of N arbitrary grains, the number of ways to arrange e grains into a cell of order e depends only on the grains shapes. By and large, our results seem to support to this argument. However, we observe a small, but systematic, μ -dependence of $P(v|e)$ for $e > 6$. We believe that this is due to effects of mechanical stability on cell shapes. This issue is tangential to the thrust of this work and will be discussed elsewhere.

Significantly, we find that friction and initial states can also be scaled away for $P(v|e)$ – all the conditional PDFs collapse under scaling the quadron volumes by the mean $v_e \equiv \int v P(v|e) dv$. The collapsed forms exhibit distinct differences for the different DSDs (Fig. 6): the flatness and the finite support of the uniform DSD give rise to a flatter maximum and a tail cutoff. The tail dependence on the DSD suggests that $P(v|e)$ cannot have a universally exponential tail. Combined with (3), this means that the observed exponential tail of $P(v)$ *must* originate in $Q(e)$.

The PDF $Q(e)$ is central to understanding the structure[15]. Its mean, \bar{e} , is related to \bar{z} via Euler's topological relation for planar graphs[16],

$$\bar{e} = \frac{2\bar{z}}{\bar{z}-2} + O\left(\frac{1}{\sqrt{N}}\right); \bar{z} = \frac{2\bar{e}}{\bar{e}-2} + O\left(\frac{1}{\sqrt{N}}\right) \quad (4)$$

The rightmost terms are boundary corrections, whose negligibility we verified in our numerical systems. $Q(e)$ depends on the friction through its sensitivity to the value of \bar{z} , while $P(v|e)$ has been shown to be hardly dependent on μ [14]. Using insight from relation (4), we find that all the $Q(e)$ curves collapse when plotted as $Q(e' = \frac{e-2}{\bar{e}-2})$ for both the log-normal and uniform DSDs (Fig. 7). Both the collapsed PDFs are fit well by a Γ distribution of the form (2), with $\alpha \approx 4$, which is only slightly different than the value observed for $P(u)$. This similarity may suggest that the exponential tail of $P(u)$ is dominated by $Q(e)$ and is much less affected by $P(v|e)$.

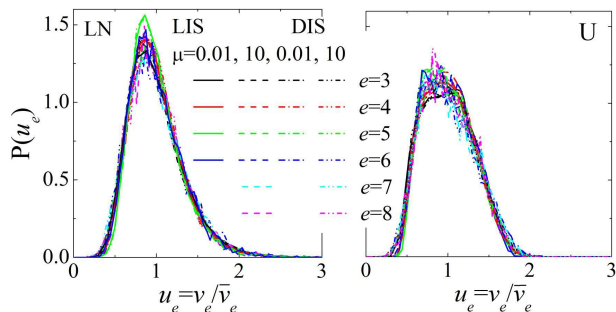


FIG. 6. The collapse of the conditional PDFs of the normalized quadron volumes for all the systems for log-normal (left) and uniform (right) DSD.

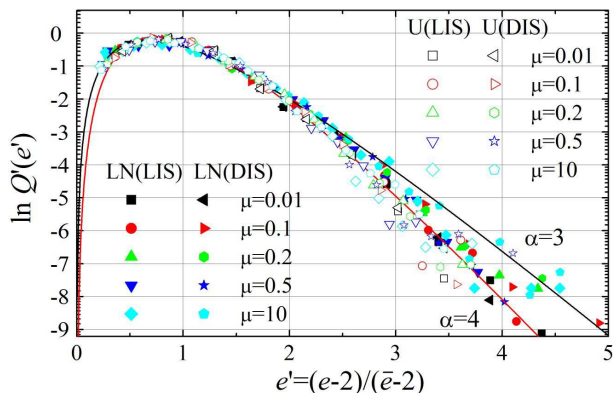


FIG. 7. The apparent collapse of all the PDFs of normalized cell orders, $Q'(e')$, $e' = (e-2)/(\bar{e}-2)$, for log-normal and uniform DSD, compared with two Γ PDFs with $\alpha = 3$ and 4.

To conclude, we have studied the effects of intergranular friction, initial state and disc size distribution, on the structural characteristics of 2D granular systems. First, we demonstrated that, for our systems, there is a universal relation between the the mean coordination number and the rattler-free packing fraction. This relation is

independent of the intergranular friction coefficient and of the initial state of the packing process, parameters that have been believed previously to affect strongly this relation. Since the rattler-free structure carries the internal stress, this finding suggests that the universality is a result of the self-organisation of the granular system under the forces generated in the packing process. Next, we used the quadron description to quantify the grain-scale structure by focusing on the statistics of two variables: the quadron volumes v and the cell order e . We found that we can scale the total and conditional distributions of these variables, so that each collapses to a universal form, apparently independent of the friction coefficient and initial state. The collapsed forms depend, however, on the DSD. We also believe that these depend on the specific packing process. We demonstrated that the exponential tail of the quadron volume PDF, which can be shown to be directly related to the "compactivity" in the statistical mechanical description of granular systems[1, 7, 17], most likely originates in $Q(e)$.

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