Local origin of global contact numbers in frictional ellipsoid packings

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In particulate soft matter systems the average number of contacts $Z$ of a particle is an important predictor of the mechanical properties of the system. Using X-ray tomography, we analyze packings of frictional, oblate ellipsoids of various aspect ratios $\alpha$, prepared at different global volume fractions $\phi_g$. We find that $Z$ is a monotonously increasing function of $\phi_g$ for all $\alpha$. We demonstrate that this functional dependence can be explained by a local analysis where each particle is described by its local volume fraction $\phi_l$ computed from a Voronoi tessellation. $Z$ can be expressed as an integral over all values of $\phi_l$: $Z(\phi_g, \alpha, X) = \int Z_0(\phi_l, \alpha, X) P(\phi_l|\phi_g) \, d\phi_l$. The local contact number function $Z_0(\phi_l, \alpha, X)$ describes the relevant physics in term of locally defined variables only, including possible higher order corrections $X$. The conditional probability $P(\phi_l|\phi_g)$ to find a specific value of $\phi_l$ given a global packing fraction $\phi_g$ is independent of $\alpha$ and $X$. An important step in defining $Z_0(\phi_l, \alpha, X)$ is the determination of the local surface area fraction $\psi_l$.

The average number of contacts $Z$ that a particle forms with its neighbors is the basic control parameter in the theory of particulate systems known as the jamming paradigm [1, 2] where $Z$ is a function of the difference between the global volume fraction $\phi_g$ and some critical value $\phi_c$. For soft, frictionless spheres a practical example would be an emulsion (this is indeed a good description) because additional contacts are formed by the globally isotropic compression of the particles which also increases $\phi$. However, in frictional granular media such as sand, salt, or sugar the control of $\phi$ is not achieved by compression but by changing the geometric structure of the sample; if we want to fill more grains into a storage box we do not compress them with a piston, but we tap them a couple of times on the counter top.

But if $Z$ and $\phi_g$ are not simultaneously controlled by a globally defined parameter such as pressure, the idea of a function $Z(\phi_g)$ runs into an epistemological problem: contacts are formed at the scale of individual particles and their neighbors. At this scale the global $\phi_g$ is not only undefined; it would even be impossible for a particle scale demon to compute $\phi_g$ by averaging over the volume of the neighboring particles. The spatial correlations between Voronoi volumes [3, 4] would require it to gather information from a significantly larger volume than the direct neighbors.

Presently, only two theoretical approaches have studied $Z$ from a local perspective: Song et al. [7] used a mean-field ansatz to derive a functional dependence between $Z$ and the Voronoi volume of a sphere. This ansatz has recently been expanded to arbitrary shapes composed of the unions and intersections of frictionless spheres [8, 9]. Secondly, Chusel et al. [10, 11] developed the granocentric model which predicts the probability distribution of contacts in jammed, polydisperse emulsions. The applicability of the granocentric model to frictional discs has been shown in [12].

The aim of this experimental study is to go beyond spheres and understand how the average $Z$ in packings of frictional ellipsoids originates from the local physics at the grain level. We find that, to a first approximation, this local physics is based on only two parameters: the material parameter $\alpha$ which is the length ratio between the short and the two (identical) long axes of the ellipsoids, and a parameters that characterize the cage formed by all the neighboring particles. We express our final result using the local volume fraction $\phi_l$, which is the particle volume divided by the volume of its Voronoi cell. However, we also show that the local area fraction $\psi_l$, which is the particle surface area divided by the surface area of its Voronoi cell, might be even more fundamental.

Frictional ellipsoids used in experiments [13, 14] exhibit a number of differences to the frictionless ellipsoids often studied numerically [15, 20]. The latter have been found to form packings with less than the number of contacts required for isostaticity, which is defined as having enough constraints to block all degrees of freedom of the particles [15, 19, 21]. This apparent paradox has been resolved by Donev et al. [22], who showed that in this analysis the contacts can not be treated as the contacts between frictionless spheres: the curvature of the ellipsoids blocks rotational degrees of freedom even in the absence of friction. In contrast, we find packings of frictional ellipsoids to be hyperstatic over the whole range of $\phi_g$ studied, which is in agreement with numerical simulation including friction [23, 24].

Particles and preparation.- Two different types of oblate ellipsoids have been studied, their properties are summarized in table I. Figure 1 a) shows pharmaceutical placebo pills (PPP) with $\alpha = 0.59$ produced by Weimer
### Table I. Material properties of the particles. The first column displays the color code used in figures 1c–d. Error-bars on µs are standard deviations over 15 experiments. The last column indicates on how many particles our analysis is based.

| aspect ratio α | half axis [mm] | type | friction coefficient µs | particles in core region |
|----------------|----------------|------|--------------------------|-------------------------|
| spheres        |                | 3DP  | 0.75 ± 0.07              | 660-850                 |
| 0.80           | 2.65           | 3DP  | 0.75 ± 0.05              | 750-850                 |
| 0.60           | 2.60           | 3DP  | 0.67 ± 0.03              | 620-730                 |
| 0.59           | 2.15           | PPP  | 0.38 ± 0.05              | 850-910                 |
| 0.40           | 1.60           | 3DP  | 0.67 ± 0.05              | 620-730                 |

Pharma GmbH. Due to their sugar coating, their surface is rather smooth; their static coefficient of friction µs against paper is 0.38 (measured using a small sledge on a slowly raised inclined plane). The second particle type displayed in figure 1b are gypsum ellipsoids cured with resin, produced with a 3D printer (Zprinter 650, Z corporation). The aspect ratio of these 3DP particles ranges from 0.4 to 1 (i.e. spherical), their rougher surface results in values of µs between 0.67 and 0.75. Due to the production process, the 3DP particles have hummocks of up to 100 μm on their short axis. As a consequence their volume deviates up to 3% from a perfect ellipsoid, compared to 1% for the PPP particles.

Samples are prepared by first creating a loose packing of ellipsoids inside a plexiglass cylinder with an inner diameter of 104 mm; then the majority of the samples is tapped in order to increase φg to the desired value. We use three different methods to prepare the initial loose samples, they are indicated by different symbols in the figures below. However, our results seem not to depend on the details of this initial preparation, details of which can be found in the supplemental material. Except for the loosest samples, the packings are compactified by applying sinusoidally shaped pulses on an electromagnetic shaker (LDS V555). The width of the pulses is 50 ms and the peak acceleration 2 g (where g = 9.81 m/s²). At a repetition rate of 3 Hz up to 1500 taps are applied to prepare the highest values of φg.

**Image analysis.** Tomograms of the prepared packings are acquired using X-ray computed tomography (GE Nanotom) with a resolution of 64 μm per voxel. The resulting three-dimensional gray scale image is the starting point for the identification of all particle centers and orientations (c.f. figure 1d) using the methods described in [25]. To reduce boundary effects, only particles with centers that are at least two long axes away from the container walls were included in our analysis; table lists the numbers of these core particles. To assure spatial homogeneity, we discard all experiments where the standard deviation of the azimuthally averaged volume fraction is larger than 0.66%. Similarly, to exclude packings with a too large degree of local order we only consider samples with θ > 0.5 rad where θ is the average angle of the short axis with respect to gravity (see supplemental material). The particle positions and orientations of all experiments reported here can be downloaded from the Dryad repository [26].

From the geometrical representation of the sample we determine the average Z using the contact number scaling method [25]. Finally, the Voronoi cells of the particles are computed with the algorithm described in [27]. Figure 1(d) displays the Voronoi tessellation of a small subset of particles. By dividing the volume of the particle by the volume of the Voronoi cell we obtain for each particle its local volume fraction φg; the harmonic mean of all particles in the core region corresponds to the global volume fraction φg. Similarly, we compute the local area fraction ψg from the surface area of the particle and its Voronoi cell; the harmonic mean corresponds to the global area fraction ψg.

The average contact number Z as a function of φg and ψg is displayed in figure 2. While ψg has received little attention in the granular community up to now, it provides clearly a better collapse for the different particle types than φg. The main conclusion of figure 2 is therefore that from a global perspective the functional dependence of Z can be written either as \( Z(\phi_g, \alpha) \) or \( Z(\psi_g) \). As expected for frictional particles, the contact number of all samples is significantly above the isostatic value of four [28]. Additionally, there is no discernible influence of the method used for the initial preparation.

**Switching to a local ansatz.** As discussed in the introduction, the formation of contacts between particles needs to be explained solely by parameters which are well defined on the particle level. In order to understand the function \( Z_l \), which describes how the contact number of a given particle depends on its local environment, we determine the local contact number for each ellipsoid. First all particles are dilated to their actual size according to its neighbors is counted.

Figure 3(b) indicates that the surface area fraction is
local contact number function $Z_l$
average contact number $Z$
local area fraction $\Psi_l$
spheres
$\alpha = 0.80$
$\alpha = 0.60$
$\alpha = 0.59$
$\alpha = 0.40$
funnel
horizontal grid
fluidized

FIG. 2. Contact number as a function of the global volume fraction and the global surface area fraction. Straight line fits are only guides for the eye. The different symbols indicate preparation of the initial packing, which is then compactified for all but the loosest samples by tapping. Given the experimental scatter $Z(\psi_g)$ displays a reasonable collapse for the different values of $\alpha$.

FIG. 3. Dependence of the local contact numbers $Z_l$ on the local area fraction $\psi_l$ for different values of $\alpha$. Curves are averaged over all experiments displayed in figure 2 using a bin size of 0.02. For the individual curves see the supplemental material.

FIG. 4. The local area fraction depends linearly on the local volume fraction. The slope is $\approx 0.75$ for all curves, the offset depends on $\alpha$. Each line corresponds to one of the experiments shown in figure 2.

the important variable. Therefore we start by computing $Z_l^*(\psi_l)$ which is displayed in figure 3. Again the collapse is reasonable, but not perfect. This suggests that $Z_l^*(\psi_l)$ is only a first order approximation. The full description $Z_l^*\left(\psi_l, X\right)$ might depend on further locally defined variables $X$ such as friction, fabric anisotropy, or measures of local order (such as the orientation $\theta$ discussed in the supplemental material). However, within the resolution of our experiment we are not able to discern between these different options.

Based on this result we can now write down a general ansatz for $Z$:

$$Z(\psi_g, \alpha, X) = \int Z_l^*(\psi_l, X) P(\psi_l|\psi_g, \alpha, X) \, d\psi_l \quad (1)$$

where $P(\psi_l|\psi_g, \alpha, X)$ is the conditional probability of finding a specific value of $\psi_l$ in a sample of particles described by $\alpha$ and potentially other parameters $X$ and prepared at a global $\psi_g$. However, contrary to $\phi_g$ which can be computed from the number of particles contained in a given volume, $\psi_g$ can not be determined from simple measurements of global variables. Which renders eq. 1 unusable in most real world situations.

This problem can be solved by a change in variables. Figure 4 shows the linear relationship between $\psi_l$ and $\phi_l$ where only the offset but not the slope depends on $\alpha$. Using this result we can rewrite our ansatz as:

$$Z(\phi_g, \alpha, X) = \int Z_l^*(\psi_l(\alpha, \phi, X)) P(\phi_l|\phi_g, \alpha, X) \, d\phi_l \quad (2)$$

with $P(\phi_l|\phi_g, \alpha, X)$ being the conditional probability to find a particle with $\phi_l$ in a given packing.

Properties of the local volume fraction distribution.– Figure 5 reveals a number of interesting scaling prop-
provide empirical guidance in developing such a theory. However, the experimental scatter in these figures does not allow us to assess the role or even necessity of the higher order correction $X$. The need for inclusion of such a parameter can also stem from the history-dependent behavior of frictional particles. It has recently been shown for spheres [30] and tetrahedra [31] that for identical $\phi_g$ the contact number can depend on the preparation history; modeling such behavior will require the addition of further locally defined parameters.

Please note that without a better understanding of the origin of the scaling properties shown in figure 5 it is not possible to decide on the causality between $\phi_l$ and $\phi_g$. So writing $P(\phi_l|\phi_g)$ can imply either that $\phi_g$ is the cause of the observed $P(\phi_l)$ or that $\phi_g$ can be seen to follow from the prepared $P(\phi_l)$.

**Conclusions.** – The global contact numbers of packings of frictional spheres and ellipsoids can be explained by an ansatz which combines a contact function which depends only on parameters defined on the particles scale and a conditional probability to find a particle with a specific value of these local parameter. The contact function assumes an especially simple, but still analytically unknown form when expressed using the local area fraction of the particles. Alternatively, it can be expressed using the local volume fraction and the aspect ratio of the particles. This demonstrates, that $\phi_g \approx 0.625$ the probability of finding a specific value of $\phi_l$ does not depend on $\alpha$. In figure 5(b) a rescaled $P$ is plotted for all values of $\phi_g$. This demonstrates, that the mean (aka $\phi_g$) and the standard deviation of the local volume fractions $\sigma(\phi_g)$ are sufficient to describe $P$. This result has previously only been known for spheres [29] and discs [12]. Finally, figure 5(c) demonstrates that the standard deviation of the local packing fraction distribution $\sigma(\phi_l)$ depends only on $\phi_g$ not $\alpha$.

Together, these results show that $P(\phi_l|\phi_g,\alpha, X)$ in equation 2 can be replaced by $P(\phi_l|\phi_g)$. Substituting $Z_l$ for $Z_l(\psi_l)$ we obtain our final result:

$$Z(\phi_g,\alpha, X) = \int Z_l(\phi_l,\alpha, X) P(\phi_l|\phi_g) \, d\phi_l \quad (3)$$

The advantage of this ansatz is a clear separation of the contact number problem into the local physics at the grain level and a probabilistic term connecting the local and the global volume fraction.

While we can not offer an analytic expression for $Z_l(\phi_l,\alpha, X)$, the results displayed in figures 3 and 4 will
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