Jamming of frictional tetrahedra

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We prepare packings of frictional tetrahedra with volume fractions \( \phi \) ranging from 0.470 to 0.612 using three different experimental protocols under isobaric conditions. Analysis via X-ray microtomography reveals that the contact number \( Z \) grows with \( \phi \), but does depend on the preparation protocol. While \( Z \) saturates at high packing fraction, the number of constraint per particle \( C \) increases further, supported by an increasing number of edge-to-face and face-to-face contacts. Even the loosest packings are strongly hyperstatic i.e. mechanically over-determined with \( C \) approximately twice the degrees of freedom each particle possesses.

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**FIG. 1.** From left to right: Close-up view of the surface of an experimental tetrahedra packing; Rendering of X-Ray Computed-Tomography data; Detected tetrahedra, colored by orientation. (Color online)

**Introduction.** – The jamming paradigm [1, 2] provides an unified viewpoint on the onset of mechanical stability in particulate soft matter systems like wet foams, emulsion, and colloids. For such frictionless spherical particles there exists a critical volume fraction \( \phi_J \approx 0.64 \) where the system becomes isostatic, i.e. the number of constraints imposed by the contacts corresponds to the degrees of freedom of the particles. Higher densities can be achieved by increasing the pressure which leads to excess contacts; these excess contacts then determine the mechanical properties of the system.

Granular matter differs in two ways from these systems. First, its nonzero surface friction \( \mu \) allows for tangential forces at particle contacts. These result in mechanical stable packings over a full range of \( \phi \) at any given pressure. Such packings differ in their structure, not their compression. However, one can still define a meaningful distance to isostaticity [3].

Secondly, most real world granular materials like sand, sugar or soil are not spherical. Only quite recently the jamming approach been applied to frictionless ellipsoids [4, 5] and tetrahedra [6]. Tetrahedra provide besides jamming a number of other interesting packing problems like the existence of quasi crystals [7] or the quest for the densest packing [8–10], which presently is believed to be a dimer crystal with \( \phi \approx 0.8563 \) [11]. However, experimental packings of necessarily frictional tetrahedra explore a much lower range of \( \phi \) [12].

From a jamming point of view tetrahedra introduce a new element: unlike spheres they have four different types of contacts: face to face, edge to face, edge to edge, and vertex to face. Nevertheless, previous numerical results have found frictionless uncompressed packings of tetrahedra to be isostatic [6, 13, 14]; the same result has been reported by the only experiment measuring contact numbers on frictional tetrahedral dice [15].

In this letter we use X-ray tomography to determine the particle positions and orientations inside tetrahedra packings. We show that even our loosest packings are highly hyperstatic and that the contact number are in general protocol-dependent.

**Experimental setup.** – The tetrahedra particles in our study are produced by injection moulding of polypropylene, and have a side length of \( a = 7 \text{ mm} \) (see Fig. 1a). The typical radius of curvature of edges and corners is \( 150 \pm 50 \mu \text{m} \) which corresponds to 2.5% of \( a \). All particles have small mold marks on one of the 6 edges, the height of this protrusions amounts to 300 \( \mu \text{m} \) at maximum [16]. The particles have a coefficient of friction \( \mu = 0.87 \pm 0.03 \), which is measured using a tilted plane and finding the angle at which face-to-face contacts start to slide past each other.

In order to explore the structure of tetrahedral packings at different densities, we compactify them by vertical shaking. We start from initially loose packings which are prepared by filling 14406 particles via a slowly lifted funnel into a cylinder of inner diameter \( D = 104 \text{ mm} \) (\( \approx 15 a \)). This method creates packings with \( \phi \) between 0.470 and 0.477, the lowest values found in this study. An electromagnetic shaker (LDS V555) then applies sine pulses (“taps”) with a width of 50 ms and a repetition rate of 3 Hz. The peak acceleration \( A_p \) per tap is measured at the base plate of the container (Kistler 8763B) and reported in units of the dimensionless acceleration

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\[ \Gamma = \frac{A_g}{g} \text{ (where } g = 9.81 \text{m/s}^2). \]

A laser distance scanner (MicroEpsilon ILD1402) mounted on a translation stage measures the surface height profile after shaking; from this profile the corresponding \( \phi \) is computed using calibration measurements from tomographic reconstruction. This results in an accuracy of the reported \( \phi \) values of \( \pm 0.003 \). Tomograms of the prepared packings are acquired using X-ray Computed Tomography (GE Nanotom) with a tungsten target and 120 kV acceleration voltage. Each dataset comprises \( 1152 \times 1152 \times 1076 \) voxels with a resolution of 100 \( \mu \text{m}/\text{voxel}. \)

**Preparation protocols.** We use three different preparation protocols. The first one will be referred to as TAP: Starting from a loose packing, a number of taps ranging from 20 to 6400 with a constant acceleration \( \Gamma = 4 \) is applied. As Fig. 2a shows, the packing fraction increases monotonically with the number of taps. This demonstrates that the system reaches after a sufficient number of taps a history-independent steady state with a packing fraction \( \phi_{ss} \).

Our second protocol RAMP is intended to study the possible range of steady state volume fractions \( \phi_{ss} \). Following Nowak et al.\cite{15}, the tap intensity \( \Gamma \) is increased stepwise from 0.5 to 10, decreased back to 0.5, and increased to 10 again. At each step, \( 10^4 \) taps are applied and the resulting \( \phi_{ss} \) is measured. The evolution of \( \phi_{ss} \) is depicted in Fig. 2(b) and comprises the following regimes: The loose packing irreversibly compacts when \( \Gamma \) is increased from 0.5 to 3, but dilates again when the acceleration is further ramped to up \( \Gamma = 10 \), leading to \( \phi_{ss} \approx 0.55 \). Subsequently, decreasing the tap intensity down to \( \Gamma = 0.5 \) creates a dense packing with \( \phi_{ss} \approx 0.60 \). Increasing \( \Gamma \) again to 10.0 demonstrates the irreversibility i.e. no hysteresis. We refer to the end points of the reversible branch as RAMP\( \Gamma=0.5 \) and RAMP\( \Gamma=10 \) in our tomographic analysis.

The third preparation protocol VIB is inspired by epitaxial growth: particles are deposited at a rate of approx. 15/s, while continuous sine vibration at 100 Hz and \( \Gamma = 10 \) is applied; a similar method has been employed to create dense packings of ellipsoids \cite{18}. Protocol VIB creates the densest packings in our study with \( \phi = 0.612 \). Apparently the slow deposition and the continuous agitation of the surface layer enables the particles to explore more effectively the configurational phase space and thus find configurations with lower potential energy.

Our range of mechanically stable packings of \( \phi = 0.470 \) to 0.612 is in accordance with the range of \( \phi = 0.48 \) to 0.64 found by Baker and Kudrolli\cite{12} for tetrahedral dice and ceramic tetrahedral particles prepared by shaking and a water-fluidized bed. Our volume fractions are however significantly lower than the value of \( \phi \approx 0.76 \) reported by Jaoshvili et al.\cite{15}, who prepared packings of tetrahedral dice under water with an unspecified protocol. This discrepancy is unlikely due to the larger corner radius of the dice as optimal packings of weakly truncated tetrahedra (resembling the dice) do not pack denser than ideal tetrahedra\cite{19}. Judging from our experience with spheres also neither the different values of \( \mu \), nor the presence of interstitial water (c.f. \cite{20} for a demonstration of static friction under water) can explain this large difference.

**Tomography analysis.** Tomographic reconstruction of the packings allows us to investigate the geometrical properties of the packing by registering the positions and orientations of all tetrahedra. The numerical analysis of the volume data is based on an iterative two-step algorithm: firstly, the approximate positions of the particle centroids are computed through the local maxima of cross-correlation with an inscribed sphere with inradius \( R_i = a/(2\sqrt{6}) \). Secondly, the orientation and exact position of each particle are determined using a steepest ascend gradient search. Detected particles are removed from the volume and the process is repeated with randomly chosen starting positions, until no more matches are possible. This approach succeeds in detecting more than 99.8\% of all tetrahedra (final reconstruction illustrated in Fig. 1c). More details can be found in the sup-
Supplementary materials. The further analysis is restricted to an inner cylindrical region with diameter 11 $a$ and height 11 $a$, containing 5056-6051 particles (depending on $\phi$). The vertical variation of the local packing fraction in this core region is smaller than 0.002.

Structure correlations. A structural measure used both in jamming and in liquid theory is the pair correlation function $g(r)$, which counts the number of neighbors at a given distance $r$, normalized by the binning volume and the average density. Fig. 3a shows $g(r)$ for a range of $\phi$. The first peak is located at $r = 0.44a$ (dashed line) and grows monotonely towards denser packings, indicating an increase of face-to-face contacts.

The peak location is close but not identical to the minimal possible distance of $2R_i = r_{min} \approx 0.408a$. Unlike the $g(r)$ of sphere packings, the left shoulder of the first peak has intrinsically a finite slope. This feature is a consequence of the lower probability of perfect face-to-face alignment compared to slightly shifted or tilted face-to-face contacts. One consequence of this specific shape of the peak is that compressed packings of soft tetrahedra will not show the same square root scaling of contact number with volume fraction as observed in sphere packings [2].

$g(r)$ decays quickly after the first peak, showing no long-range translational ordering. This is in contrast to the $g(r)$ obtained from Monte Carlo (MC) simulations of tetrahedra [14, 13] which revealed long-range structure at densities as low as $\phi = 0.46$. The difference can be explained by the preparation: the MC simulations prepare packings without gravity and friction by slow compression of a liquid phase. In contrast our frictional samples start to jam due to gravity at $\phi \approx 0.47$, after which geometric frustration and pressure in the pile restrict further alignment.

The orientational order can also be quantified with an angular correlation function $F(r)$ (depicted in Fig. 3b), which measures the relative orientation of face normals. $F(r)$ reaches 180° for a perfect face-to-face configuration and 150° for a random configuration. While the translational order in $g(r)$ decays quickly, the behavior of $F(r)$ suggests long-range orientational order, particularly for the densest packings. This result is again in disaccord to the findings in [15] but agrees with the numerical results in [2].

Contact numbers. In order to study the origin of mechanical stability, we determine the average contact number $Z$ of the tetrahedra. As we can not distinguish real contacts from close neighbors based on local force measurements [21], we determine $Z$ from a model based fitting method introduced by Aste et al. [22] for sphere packings. The supplementary material provides more details on this approach which does account for the finite resolution of tomography and detection.

The resulting contact numbers at different densities and for the different preparation protocols are shown in Fig. 4. The packings prepared by TAP show $Z$ increasing monotonely with $\phi$. The contact numbers of the two densest packings, RAMP($\Gamma=0.5$) and VIB, remain constant compared to the densest TAP sample. However, the packings prepared by RAMP($\Gamma = 10$) deviate distinctly: For comparable $\phi$, contact numbers are approx. 0.5 lower, confirming the influence of the preparation protocol. Also the initial loose packings show variations in $Z$ of the order 0.5.

Constraints. Contrary to spheres, $Z$ is not sufficient to evaluate the distance to isostaticity, because the number of mechanical constraints fixed by a contact depends on the specific contact geometry. Tetrahedra have 4 different types of contacts: face-to-face (F2F) contacts, which are mechanically equivalent to 3 individual point contacts, edge-to-face (E2F) contacts (equivalent to two point contacts) and the vertex-to-face (V2F) and edge-to-edge (E2E) contacts which correspond to a single point contact. For considering the mechanical stability, we have to assign one normal force component to each point contact. Additionally, friction introduces two tangential force components shared by all the in-plane point contacts. As these force components are shared between two tetrahedra, we obtain the constraint numbers $C_{F2F} = 2.5$, $C_{E2F} = 2$, and $C_{V2F} = C_{E2E} = 1.5$. Mul-
tipplying these numbers with the according type-specific contact numbers gives the number of constraint per particle $C$. For an isostatic packing $C$ needs to be equal to the degrees of freedom each particle possesses, in the case of tetrahedra this number is $6$.

![Diagram](image)

**FIG. 5.** Top: Number of different contacts per particle as a function of packing fraction. The number of F2F and E2F contacts increases, while the point contacts (V2F and E2E) reach saturation values. Bottom: Variation of the number of constraint per particle with packing fraction. (Color online)

We determine the contact type using the adjacent face-to-face-angle $\alpha_{F2F}$ of each pair of contacting tetrahedra. We e.g. classify a contact as F2F if $\alpha_{FF}$ is in the range $176.9^\circ$ to $180^\circ$. The lower threshold of this range is based on an experimental calibration: We prepare a sample with 80 single face-to-face contacts and measure the cumulative distribution of $\alpha_{FF}$ in this particular sample. This distribution is well described by an error function with a point of inflexion at $m = 178.2^\circ$ and a standard deviation $\sigma = 1.3^\circ$, suggesting an optimal threshold at $m - \sigma$. Please see the supplementary material for full data and methods.

Figure 5 shows that the number of F2F and E2F contacts increases monotonely with $\phi$. At the same time the point-like contacts E2E and V2F exhibit a maximum around $\phi = 0.52$ or saturate after an initial increase. The number of constraints per tetrahedra is between 11 and 15 and therefore much higher than the isostatic limit of 6. While this result does not contradict the isostatic packings found in simulations of frictionless tetrahedra 6,13,14, there is a clear disagreement with the experiments using frictional dice reported in 15. There, however, the authors use the contact-specific constraint numbers pertinent to frictionless particles. If the contacts are treated as frictional, the result will also be a hyperstatic packing. See also the discussion in 13.

**Conclusion.** We have shown that frictional tetrahedra packings exhibit a hyperstatic constraint number $C$. While the geometry-independent contact number $Z$ saturates at $\phi \approx 0.59$, the number of constraints $C$ grows further, attributable to point contacts being transformed into face-to-face and edge-to-face contacts. We find the values of $C$ and $Z$ to depend both on packing fraction and on preparation history. Our experiments involve non-spherical particles and consider friction explicitly, thus providing experimental support for extending the jamming paradigm. Further work will address different preparation methods to increase the packing fraction, and investigate local structures, as $F(r)$ of dense packings indicates structures beyond nearest neighbors.

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