Compression- and Shear-Driven Jamming of U-Shaped Particles in Two Dimensions

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We introduce a dynamic numerical model for simulating soft, U-shaped, frictionless particles in $d = 2$ dimensions and explore the jamming transition of such particles under uniform compression and shearing. Upon slow compressing, the onset of jamming occurs when the average particle contact number reaches the isostatic value for frictionless asymmetric particles, $z_{\text{iso}} = d(d+1) = 6$, and is characterized by a pressure which increases roughly linearly with packing fraction. Under driven steady state shearing, jamming occurs at a higher packing fraction than observed in compressing.

I. INTRODUCTION

Granular materials are found frequently in natural and industrial settings with a wide variety of different types of constituent particles. Considerable theoretical and numerical work has investigated the jamming transition in such granular systems [1–3]. Most work has focused on the simplest case of spherical and circular particles [4–8]. Some recent work has considered ellipsoidal particles [9–14]. However it remains of interest to explore the effects that more complex particle shape may have on behavior in granular materials, and in particular on the jamming transition.

Several recent works have explored the behavior of U-shaped particles, i.e. “staples” (see Fig. 1), which are interesting because their concave shape allows them to interlock, creating an effective inter-particle cohesion. In one study, this geometric cohesion was exhibited through the formation of free-standing columns of staples [15]. When allowed to collapse under vibration, the column height followed a stretched exponential, and the effective cohesion governing the rate of collapse was found to have a maximum value which depended on the spine to barb ratio of the staples.

In this work we use numerical simulations of a two dimensional system of frictionless U-shaped staples to explore whether such geometric cohesion has any significant effects on the jamming transition. We consider both uniform compression-driven jamming and uniform shear-driven jamming. We investigate the response of the pressure in the system to different fixed compression and shear rates, and relate the onset of jamming to the isostatic condition [16] on the average particle contact number ($z$).

II. MODEL

Our model consists of a system of $N = 1024$ identical frictionless staples in a two dimensional square box of side length $L$. Particles in contact interact with a repulsive elastic force. As contact detection for arbitrarily shaped particles is in general difficult, we model our staples as a rigid composite of three orthogonal spherocylinders, as illustrated in Fig. 1. For spherocylinders, an efficient contact algorithm is known [17]. The geometry of such staples are determined by their diameters $D$ and axis lengths $A$, which determine the composite staple’s spine length $w$ and barb length $\ell$.

![FIG. 1. The geometric model for a staple used in simulations consisting of three spherocylinders. The spherocylinders are characterized by their diameters $D$ and axis lengths $A$, which determine the composite staple’s spine length $w$ and barb length $\ell$.](image)

As contact detection for arbitrarily shaped particles is in general difficult, we model our staples as a rigid composite of three orthogonal spherocylinders, as illustrated in Fig. 1. For spherocylinders, an efficient contact algorithm is known [17]. The geometry of such staples are determined by their diameters $D$ and axis lengths $A$. All spherocylinders in this work are congruent, with an axis to barb ratio of $A/D = 4/1$, giving all of the resulting staples a spine length $w = A + 2D$, barb length $\ell = A$, and barb to spine ratio of $\ell/w = 2/3$. This is slightly higher than the ratio found for maximum cohesiveness in three dimensional columns [15]. We will assume that the staples have a total mass $m$ distributed uniformly over the area of the spherocylinders. The packing fraction $\phi$ of the system is given by,

$$\phi = NA/L^2, \quad A = 3DA + 3\pi(D/2)^2,$$  \hfill (1)

with $A$ the area of a single staple.

Defining $r_{ab}$ as the shortest distance between the axes of two spherocylinders $a$ and $b$, we use an harmonic interaction for the elastic energy of two spherocylinders in contact,

$$U^e(r_{ab}) = \begin{cases} -\frac{1}{2} k_e (1 - |r_{ab}|/D)^2, & |r_{ab}| < D \\ 0, & |r_{ab}| \geq D \end{cases},$$ \hfill (2)
with repulsive force $\mathbf{F}_{ab}^{el} = -dU_{ab}^{el}/d\mathbf{r}_{ab}$ acting at the point on the axis which is an endpoint of $\mathbf{r}_{ab}$. This force is directed in the outward direction normal to the surface. The total elastic force acting at the center of mass $\mathbf{r}_i$ of staple $i$ is then the sum of all contact forces acting on its constituent spherocylinders,

$$\mathbf{F}_{i}^{el} = \sum_{\text{contacts } ab} \mathbf{F}_{ab}^{el},$$

and the total torque about the staple’s center of mass from these elastic forces is,

$$\tau_{i}^{el} = \sum_{\text{contacts } ab} \hat{z} \cdot (\mathbf{r}_{iab} \times \mathbf{F}_{ab}^{el}),$$

where $\mathbf{r}_{iab}$ is the displacement from the staple’s center of mass $\mathbf{r}_i$ to the contact point $ab$ on the spherocylinder axis, and $\hat{z}$ is the unit normal perpendicular to the plane of the staples.

In addition to elastic contact forces, the staples also experience a viscous dissipative force. Following a commonly used simple model [518], we take this dissipative force to be proportional to the difference between the local velocity of each element of the staple and an average background velocity $\mathbf{v}_{av}(r)$. We may think of this background $\mathbf{v}_{av}(r)$ as representing either the average velocity of other staples at position $r$, or as the velocity of a host fluid in which the staple is embedded. If $\mathbf{v}_i \equiv \dot{r}_i$ is the velocity of the center of mass of staple $i$, and $\omega_i \equiv \dot{\theta}_i$ is its angular velocity about the center of mass, then the dissipative force per unit area acting at point $\mathbf{r}_i + \mathbf{r}'$ on the staple (where $\mathbf{r}'$ is the position relative to the center of mass $\mathbf{r}_i$) is,

$$\mathbf{f}_{i}^{\text{dis}}(\mathbf{r}') = -k_d \left[ \mathbf{v}_i + \omega_i \hat{z} \times \mathbf{r}' - \mathbf{v}_{av}(\mathbf{r}_i + \mathbf{r}') \right].$$

The total dissipative force acting at the staple’s center of mass is then

$$\mathbf{F}_{i}^{\text{dis}} = \int_{\text{staple}} d\mathbf{r}' \mathbf{f}_{i}^{\text{dis}}(\mathbf{r}')$$

where $\mathbf{r}'$ integrates over the area of the staple. The total dissipative torque on the staple is,

$$\tau_{i}^{\text{dis}} = \int_{\text{staple}} d\mathbf{r}' \hat{z} \cdot [\mathbf{r}' \times \mathbf{f}_{i}^{\text{dis}}(\mathbf{r}')] .$$

To model a system uniformly compressed at a fixed rate $\epsilon$, we take as the average background velocity

$$\mathbf{v}_{av}(r) = -\epsilon \mathbf{r}$$

and use periodic boundary conditions on a box of length $L$ that shrinks at the same rate, $\dot{L} = -\epsilon L$. Using $\int d\mathbf{r}' = A$, $\int d\mathbf{r}' \mathbf{r}' = 0$, and defining,

$$I \equiv \int_{\text{staple}} d\mathbf{r}' |\mathbf{r}'|^2 / A,$$
packing fraction $\phi = 0.2$. Initial states are chosen to have zero energy by placing staples one-by-one at random positions and orientations, rejecting placements which result in any staple overlaps. This allows us to prepare random systems without physically unrealistic effects such as staple axes penetrating through each other (see Fig. 2). Our results are averaged over at least 10 independent runs starting from different zero-energy configurations.

Figure 3 shows the elastic part of the pressure $p$, calculated from the trace of the elastic stress tensor in the usual way, vs packing fraction $\phi$, for several different compression rates $\epsilon = 1 \times 10^{-5}$ to $5 \times 10^{-8}$. As $\phi$ increases, $p$ increases from zero. As the compression rate $\epsilon$ decreases, the low-$\phi$ tail of $p$ sharpens up to give a jamming transition at $\phi_J \approx 0.49$. As $\phi$ increases above $\phi_J$, pressure $p$ increases roughly linearly as has been found previously for frictionless disks and spheres with a harmonic interaction [1].

Jamming is often associated with the condition of isostaticity, when the total number of degrees of freedom exactly equals the total number of constraints from the contact forces [16]. For frictionless particles, where contact forces are always normal to the surface at the point of contact, the isostatic condition is given by $N d_J = N z_{iso}/2$, so $z_{iso} = 2d_J$. Here $d_J$ is the number of degrees of freedom per particle and one notes that each contact is shared by two particles. For spherically symmetric particles, which are invariant under rotation, only center of mass motion is relevant, so $d_J = d$ and $z_{iso} = 2d$. While frictionless disks and spheres have been clearly demonstrated to be isostatic at the jamming $\phi_J$ [3], ellipsoidal particles have been found to be hypostatic at jamming, $\langle z \rangle < 2d_J$ [11, 14]. It has further been argued that smooth convex shaped particles will in general be hypostatic at jamming [12, 20]. However our staples are concave, and so it remains in question whether isostaticity describes the state of staples at jamming.

For particles with no rotational symmetries, such as our staples, there are $d_J = d(d+1)/2$ total translational and rotational degrees of freedom per particle [20]. Thus the isostatic condition for our staples in $d = 2$ dimensions is $z_{iso} = 2d_J = 6$. Note that, since our particles are concave, the same two neighboring staples may contact each other at more than one point, and in fact may share up to 4 different contacts. Therefore the average number of contacts per staple $\langle z \rangle$, in general greater than the average number of neighbors each staple is in contact with, has been observed for other non-convex particles [21].

In Fig. 3 we show $\langle z \rangle$ vs $\phi$ as we compress with different rates $\epsilon$. Comparing the curves of $\langle z \rangle$ against the curves of pressure $p$, we see that isostaticity $\langle z \rangle = 6$ does indeed seem to hold at the jamming transition $\phi_J \approx 0.49$. By fitting the linear portion of the pressure curve at our smallest compression rate $\epsilon = 5 \times 10^{-8}$, and extrapolating to zero, we find that $\phi_J$ where this pressure vanishes agrees with the isostatic packing fraction where $\langle z \rangle = 6$.

We have also found that the jamming packing fraction $\phi_J$ depends slightly on the initial packing fraction at which the zero-energy configurations are prepared. Systems which were initialized at very dilute packing fractions, $\phi \leq 0.2$, all jammed at the same $\phi_J \approx 0.49$. However, when the packing fraction of the initial state increased, the subsequent jamming $\phi_J$ also slightly increased. For configurations prepared at an initial $\phi = 0.3$, a $\phi_J \approx 0.5$ was observed. A similar dependence of $\phi_J$ on the ensemble of initial states from which compression begins was found for frictionless spheres and disks [22, 23].
We now consider the jamming of the staples under the application of a uniform applied shear strain rate \( \dot{\gamma} \). We start the system off at a given packing fraction \( \phi \) in the interval \([0.45, 0.59]\), and shear at fixed \( \phi \) for a range of strain rates \( \dot{\gamma} = 2 \times 10^{-4} \) to \( 2 \times 10^{-6} \). For each value of \( \phi \) and \( \dot{\gamma} \) we initialize the system by starting with a different zero-energy configuration at a dilute packing fraction, and then compressing to the desired packing fraction \( \phi \) before shearing. While we expect that the system, when sheared long enough, will eventually lose memory of its initial configuration [23], we find that memory of the initial configuration, particularly at denser \( \phi \) and slower \( \dot{\gamma} \), can persist for quite long strains. Many systems did not reach a steady state until after a total strain of \( \gamma = \dot{\gamma} t > 150 \). Our results are averaged over a total strain \( \gamma \geq 100 \) after the system has reached steady state.

In Fig. 4 we show the resulting steady-state average of the pressure \( p \). As with compression, we find that systems sheared at slower rates show pressure curves that shift towards higher packing fractions \( \phi \). In the limit \( \dot{\gamma} \rightarrow 0 \), the measured \( p \) represents the pressure along the yield stress curve; we expect in principle to see \( p \) vanish for all \( \phi < \phi_J \), and then rise to finite values above \( \phi_J \). However, unlike our compression results, we are unable to shear at slow enough rates to see such a convergence to the \( \dot{\gamma} \rightarrow 0 \) limit. It is thus difficult to estimate the precise value of the shear-driven jamming \( \phi_J \). Our data are not accurate enough, nor our system large enough, to do a critical scaling analysis to determine \( \phi_J \), as has been done for the case of frictionless disks [24].

If we believe that, as in compression, shear-driven jamming will occur when the system satisfies the isostatic condition, then we see from the plot of \( \langle z \rangle \) vs \( \dot{\gamma} \) in Fig. 4 that, for our different shear rates \( \dot{\gamma} \), this occurs when \( 0.54 < \phi < 0.57 \), with the largest \( \phi \) occurring at the slowest \( \dot{\gamma} \). Comparing with Fig. 3 (note vertical dashed lines) we see that, for each value of \( \dot{\gamma} \), this roughly corresponds to the \( \phi \) at which the pressure increases above its small \( \phi \) tail to rise linearly.

As another attempt to look for the limiting \( \dot{\gamma} \rightarrow 0 \) behavior, and so determine \( \phi_J \), we plot in Fig. 5 the pressure analog of viscosity \( p/\dot{\gamma} \) vs \( \dot{\gamma} \) at various fixed values of \( \phi \). We expect that \( p/\dot{\gamma} \) will saturate to a finite value as \( \dot{\gamma} \rightarrow 0 \) for all \( \phi < \phi_J \). But since above \( \phi_J \) the system supports a finite stress even as the shear rate approaches zero, we expect \( p/\dot{\gamma} \) must diverge as \( \dot{\gamma} \rightarrow 0 \) for \( \phi > \phi_J \). At low \( \phi \leq 0.51 \) in Fig. 3 we clearly see the expected plateau to a finite value as \( \dot{\gamma} \) decreases. As \( \dot{\gamma} \) increases for these low \( \phi \), we see the shear thinning behavior (decreasing \( p/\dot{\gamma} \)) that is typical of overdamped, soft, frictionless granular materials [24, 25]. At higher \( \phi \) we see a continuing increase in \( p/\dot{\gamma} \) as \( \dot{\gamma} \) decreases. Our data suggests that the crossover between these two different limiting behaviors occurs at roughly \( \phi \approx 0.52 \). However one cannot say with confidence whether the curves at \( \phi > 0.52 \) will continue to increase, or may bend over to saturate to a finite value, as \( \dot{\gamma} \) decreases to smaller values than we have been able to simulate. Our value \( \phi \approx 0.52 \) should therefore be taken as a likely lower bound for the shear-driven \( \phi_J \). Though we can only give a lower bound for the shear-driven \( \phi_J \), we note that it does clearly seem to be larger than the compression-driven \( \phi_J \), as has also been found for frictionless disks [23, 26].

V. CONCLUSIONS

We have studied the jamming transition in a system of concave, frictionless, U-shaped particles under both compression and steady-state shearing. In compressed systems we found that the jamming transition is clearly associated with isostaticity, and occurs at values of \( \phi_J^{comp} \) between 0.49 and 0.5 depending on the initial packing fraction from which the compression begins. In steady-state shearing our results suggested a lower bound for
the jamming transition to be \( \phi_{J}^{\text{bear}} \geq 0.52 \). These features, that (i) compression-driven jamming occurs at the isostatic point, that (ii) compression-driven jamming is influenced by the ensemble of initial states from which the compression begins, and that (iii) shear-driven jamming occurs at a higher packing fraction than found from compressing dilute systems, are all in common with the behavior observed for the jamming of frictionless disks. The main effect that we have observed, which we attribute to our concave particle shape and the resulting geometric cohesion, is the very much longer time it takes for the system to reach steady-state, independent of the initial configuration, upon shearing.

Several works \cite{21, 27, 28} have suggested that geometric roughness on the surface of otherwise frictionless particles may provide a good model for the inter-particle tangential frictional forces that are usually present in dry granular systems. Such roughness has been modeled \cite{21} by asperities on the surface of spherical particles, leading to a concave particle surface. One may therefore ask if the concave staples studied in the present work display any of the features usually associated with the jamming of frictional particles. Our results, however, do not seem to find so.

In looking at Fig. 3, we see that the apparent jamming transition \( \phi_{J} \) moves to slightly higher values as the compression rate \( \epsilon \) decreases. Similar results have been found for frictionless spheres \cite{29, 30}. This is in direct contrast to what is observed for frictional spheres, where the slower the compression rate the lower \( \phi_{J} \) one finds \cite{31, 33}. Numerical simulations of slowly sheared frictional systems \cite{34} show a discontinuous jump in the pressure at jamming, provided the friction coefficient is not too small. Our results in Fig. 4 do not give any sign of such a discontinuous jump. We thus conclude that inter-particle friction and geometric cohesion likely play quite different roles in the phenomenological behavior of granular materials.

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**APPENDIX**

The function \( f(\theta) \) that appears in Eq. (12) for the dissipative torque on a sheared staple is,

\[
f(\theta) \equiv \int_{\text{staple}} \frac{d\mathbf{y}^2}{d|\mathbf{r}|^2},
\]

where \( \mathbf{r} \) measures the distance from the staple’s center of mass, and \( \theta \) is the angle that the staple’s spine makes with the \( \hat{x} \) axis. We will approximate this integration by treating the staple as three connected, infinitesimally thin, rods with spine having a length \( w \) and barbs each having length \( \ell \), otherwise in the same arrangement as shown in Fig. 1.

We consider first the general case of a rod of length \( L \), centered at a position \( \mathbf{R} = (X, Y) \) and oriented at an angle \( \alpha \) with respect to the \( \hat{x} \) axis, as shown in Fig. 6. If \( s \) is a coordinate that runs down the length of the rod from \(-L/2\) to \(L/2\), we then have,

\[
\int_{\text{rod}} d\mathbf{y}^2 = \int_{-\frac{L}{2}}^{\frac{L}{2}} ds \left( Y + s \sin \alpha \right)^2 = Y^2 L + \frac{L^3}{12} \sin^2 \alpha
\]

while

\[
\int_{\text{rod}} d|\mathbf{r}|^2 = \int_{-\frac{L}{2}}^{\frac{L}{2}} ds \left[ (X + s \cos \alpha)^2 + (Y + s \sin \alpha)^2 \right] = |\mathbf{R}|^2 L + \frac{L^3}{12}
\]

To apply this to our staple, we consider first the situation when the staple is oriented at \( \theta = 0 \), with the spine parallel to the \( \hat{x} \) axis and the barbs in the negative \( \hat{y} \) direction, as shown in Fig. 7. If we set the origin of our coordinates at the center of mass of the three rods comprising the staple, then the spine is centered at position

![Graph](image-url)
\begin{align*}
\mathbf{R}_s &= c \hat{\mathbf{y}}, \text{ where } c \equiv \ell^2/(w + 2\ell). \text{ The barbs are centered at positions } \mathbf{R}_{b\pm} = \pm(w/2) \hat{\mathbf{x}} + (c - \ell/2) \hat{\mathbf{y}}. \text{ Hence we have } |\mathbf{R}_s|^2 = c^2 \text{ and } |\mathbf{R}_{b\pm}|^2 = w^2/4 + (c - \ell/2)^2. \text{ When the staple is rotated through an angle } \theta, \text{ we have for the resulting } Y\text{-components, } Y_s = c \cos \theta, Y_{b\pm} = \pm(w/2) \sin \theta + (c - \ell/2) \cos \theta. \\
\text{We now apply Eqs. (17-18) to each segment of our staple, using for the spine } L_s = w, \alpha_s = \theta, \text{ and for the barbs } L_b = \ell, \alpha_b = \theta + \pi/2, \text{ and the above values of } |\mathbf{R}_s|^2, |\mathbf{R}_{b\pm}|^2, Y_s \text{ and } Y_{b\pm}. \text{ Adding the results we get,} \\
\int_{\text{staple}} d\mathbf{r} \; y^2 &= \left(\frac{w^3}{12} + \frac{w^2 \ell}{2}\right) \sin^2 \theta + \left(\frac{2\ell^3}{3} - \ell \theta^3\right) \cos^2 \theta \\
\text{and} \\
\int_{\text{staple}} d\mathbf{r} \; |\mathbf{r}|^2 &= \frac{w^3}{12} + \frac{w^2 \ell}{2} + \frac{2\ell^3}{3} - \ell \theta^2.
\end{align*}

Finally, substituting back in \( c = \ell^2/(w + 2\ell) \), we can simplify the above to write \( C \) as a function of a single variable \( b \equiv \ell/w \), the barb to spine ratio,

\begin{equation}
C = \frac{1 + 8b + 12b^2}{1 + 8b + 12b^2 + 8b^3 + 4b^4}.
\end{equation}

We note that \( C = 1 \) when \( b = 0 \) and \( C \to 0 \) when \( b \to \infty. \)
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