Granular ‘glass’ transition

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The transition from a flowing to a static state in a granular material is studied using large-scale, 3D particle simulations. Similar to glasses, this transition is manifested in the development of a plateau in the contact normal force distribution $P(f)$ at small forces, along with the splitting of the second peak in the pair correlation function $g(r)$, suggesting compaction and local ordering. The mechanical state changes from one dominated by plastic intergrain contacts in the flowing state to one dominated by elastic contacts in the static state. We define a staticity index that determines how close the system is to an isostatic state, and show that for our systems, the static state is not isostatic.

Granular materials are many-body systems which can exhibit properties of both liquids and solids, often at the same time. Features such as jamming in silos and hoppers $^4$ and heterogeneous force propagation $^3$ have motivated new proposals for constitutive relations for granular materials $^3$ in contrast to the established elasto-plastic theories $^5$. Moreover, the emerging field of “jammed systems” $^6$ seeks to understand whether analogies may be drawn between diverse systems which have the common properties that they are far from equilibrium, and unable to explore phase space.

O’Hern et al. $^8$ have recently shown that similarities exist between the properties of static granular packings and other amorphous systems; in particular, they compared force distributions for simulated systems of soft-spheres undergoing a glass transition with experimental data from static granular packings $^3$. These studies suggest that it may be interesting to consider the transition of granular materials from flowing to static, and inquire about its similarities with the glass transition. In this Letter we study the dynamic jamming transition of systems of athermal grains through large-scale simulation. In particular, we consider the behavior of dense packings of granular particles flowing down an inclined plane as the tilt angle $\theta$ is reduced through the angle of repose $\theta_r$ at which flow ceases.

The chute flow geometry we employ relies on gravity to compactify the system. Our earlier simulation studies in this geometry $^3$ have proven their reliability by reproducing key experimentally observed characteristics of dense granular flows $^3$, such as the existence of steady state flow over a range of angles between $\theta_r$ and a maximum angle of flow stability $\theta_{\text{max}}$, as well as the dependence of the angle of repose on pile height for shallow piles less than 20-30 grain diameters in depth.

The transition from flowing to static states suggests that for systems generated in this way, $\theta_r$ can be regarded as an analogue for the glass transition temperature $T_g$, and we characterise the transition by the following properties:

- $P(f)$, the probability distribution of normal forces, develops a plateau in the static state.
- The radial distribution function, $g(r)$ develops a split second peak, and growth of the first peak, indicating compaction and increased short-range ordering.
- The average co-ordination number, $z_c$, jumps discontinuously. Moreover, the static state that results when motion ceases is not isostatic.

Furthermore, we observe a significant change in the number and nature of interparticle contacts: although a finite fraction of contacts are plastic (at Coulomb yield) for all flowing piles, almost none are plastic when the pile becomes static $^3$. The average co-ordination number increases continuously towards four in the flowing state and jumps to well above four for the static packing – four being the theoretical minimal co-ordination number for a network of frictional grains.

We carried out molecular dynamics simulations in 3D on a model system of $N = 8000$ mono-disperse, cohesionless, frictional spheres of diameter $d$ and mass $m$. The system is spatially periodic in the $xy$ (flow – vorticity)-plane, and is constrained by a rough bottom bed in the $z$-direction, with a free top surface. The static packing height is about $40d$. Particles interact only on contact through a Hertzian interaction law in the normal and tangential directions to their lines of centers $^3$. That is, contacting particles $i$ and $j$ positioned at $\mathbf{r}_i$ and $\mathbf{r}_j$ experience a relative normal compression

$$\delta = |\mathbf{r}_{ij} - d|,$$

where $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$, which results in a force

$$\mathbf{F}_{ij} = \mathbf{F}_n + \mathbf{F}_t. \quad (1)$$

The normal and tangential contact forces are given by

$$\mathbf{F}_n = \sqrt{\delta/d} \left( k_n \delta \mathbf{n}_{ij} - \frac{m}{2} \tau^*_n \mathbf{v}_n \right), \quad (2)$$
Energy (KE) per particle, normalised by $\delta t = \frac{mg}{gd}$.

where $n_{ij} = r_{ij}/r_{ij}$, with $r_{ij} = |r_{ij}|$, $v_n$ and $v_t$ are the normal and tangential components of the relative surface velocity, and $k_n$ and $\gamma_n$ are elastic and viscous elastic constants respectively. $\Delta s_t$ is the elastic tangential displacement between spheres, obtained by integrating surface relative velocities during elastic deformation of the contact [10]. The magnitude of $\Delta s_t$ is truncated as necessary to satisfy local Coulomb yield criteria $F_t \leq \mu F_n$, where $F_t \equiv |F_t|$ and $F_n \equiv |F_n|$, and $\mu$ is the local particle friction coefficient.

In the steady state flow regime, changes in the particle friction $\mu$, the damping coefficients $\gamma_n,t$, or particle hardness $k_n$, do not change the qualitative nature of our findings [11]. For the present simulations, we set $k_n = 2 \cdot 10^5 mg/d$, $k_t = \frac{50 \sqrt{g/d}}{\phi}$, $\gamma_n = 0.0$, and $\mu = 0.5$ [11]. We choose a time-step $\delta t = 10^{-4} \tau$, where $\tau = \sqrt{d/g}$.

To initiate flow, we tilt the bed to a large angle ($\theta \approx 26^\circ$) long enough to remove any history effects of construction. We then lower the angle, in unit increments, to the desired value in the range for which there is steady state flow, $20^\circ \lesssim \theta \lesssim 26^\circ$ [10]. In this range, the energy input from gravity is balanced by that dissipated in collisions. We can approach the flowing angles from above and below and always obtain the same results.

Lowering $\theta$, the kinetic energy of the system decreases, however flow continues down to $\theta_{cr}(\approx 19.4^\circ)$ for the set of parameters used here [13]. As $\theta$ is reduced, the volume fraction increases, as shown in Fig. 1. We generated further static packings by taking the stopped state at $\theta = 19^\circ$ and reducing the tilt to zero. The volume fraction of the static packing for $\theta = 0.0$, $\phi = 0.599 \pm 0.005$, is less than the random close packing value $\phi_{rcp} \simeq 0.64$.

In order to investigate the distribution of contact forces in flowing and static states, we computed the probability density function (PDF) $P(f)$, where $f \equiv F_n/F_{n(z)}$ is the ratio of the normal contact force magnitude $F_n$ to its average value at the depth $z$ of each contact. Since our system is spatially periodic in the horizontal plane, with no side-walls, the pressure does not saturate with depth, requiring separate averaging at each value of $z$. The data were averaged over 1000 configurations over a period of $200 \tau$ in the steady state at each flowing angle and 5 configurations for the static states.

As shown in Fig. 2, the PDFs exhibit familiar exponential tails at high forces. When $\theta$ is reduced towards $\theta_{f}$, a plateau develops near $f = 1$ (see inset), similar to the behaviour observed in Ref. 8 near the glass transition. It may be argued on this basis that $\theta_{f}$ appears analogous to $T_g$ in a glass-former. However, the development of this feature is rather subtle in our system, and does not appear to be a sharp indicator of the transition from the flowing to the static case. Upon further relaxation of the stress by reducing $\theta$ to zero, the feature becomes more prominent similar to the results in Ref. 8.

As with glass transitions, we have found only subtle structural evidence for the transition from flow to rest. The radial distribution function $g(r)$ is fairly insensitive to the tilt angle, as shown in Fig. 3. Although there is no long range ordering, in the inset to Fig. 3 we observe the gradual splitting of the second peak as $\theta$ is reduced. The system develops more locally ordered structures as it becomes more compact [13].

More significantly, the first peak in $g(r)$ increases with decreasing $\theta$. Because particle neighbors are defined only on contact in our simulations, the first peak in the radial distribution function corresponds to the average coordination number $z_{cr}$, which correspondingly increases as $\theta$ decreases (see Fig. 3).
An important characteristic that separates the granular system from a glass forming liquid is the existence of interparticle friction and yield. To explore the influence of intergran friction, we distinguish between intergran contacts at their yield criterion \( F_i = \mu F_n \) (plastic contacts), which respond plastically to some external perturbations, from contacts with \( F_i < \mu F_n \) (elastic contacts), whose response is determined by elastic deformations of the constituent grains. Note that the relationship between plasticity/elasticity of individual contacts between grains and the mechanical response of the entire system has not been explored in this study.

We find that the nature of grain-grain contacts is quite different in the flowing and static regimes. The probability densities of frictional saturations \( \zeta \equiv F_i / \mu F_n \) are shown in Fig. 3 for various tilt angles. The fraction \( n_c \) of plastic contacts (with \( \zeta = 1 \)) decreases as the tilt angle is decreased towards \( \theta_r \) (see Fig. 4), accompanied by a decrease in the average frictional saturation of elastic contacts. For the static piles at \( \theta < \theta_r \), almost all grain contacts are elastic.

A related question is whether or not static piles of rigid grains satisfy an isostaticity condition, where the number of contacts is the minimum required to satisfy force and torque balance equations for each grain. This isostaticity hypothesis has been frequently invoked in recent theoretical work attempting to derive macroscopic constitutive relations directly from the microstates of static granular packings. Isostaticity is required for a unique determination of the individual contact forces solely in terms of the microstate. Otherwise, the details of grain deformations (for example, Hookean or Hertzian force laws) must be considered in order to determine the stress state of the pile, as the rigid grain problem becomes ill-posed.

![Radial distribution function](image)

**FIG. 3.** Radial distribution function \( g(r) \) for various tilt angles \( \theta \). The inset shows the region near the second peak.

Counting the degrees of freedom (DOF) in the contact forces suggests that isostaticity requires \( z_c = 4 \) for frictional contacts (with 3 DOF - one vector force - per contact and 6 equations per grain) and \( z_c = 6 \) for frictionless contacts (with 1 DOF - one normal force - per contact but only 3 equations per grain) for spherical grains. However, one DOF is eliminated for each frictional contact that reaches the yield criterion and becomes plastic: the magnitude of the tangential force in this case is determined by the normal force and the friction coefficient \( \mu \). Thus, if the fraction of plastic contacts is \( n_c \), for a co-ordination number \( z_c \) the total number of DOF characterizing interparticle forces is

\[
N_f = N / 2 \left[ 3(1-n_c) + 2n_c \right],
\]

and requiring \( N_f \geq 6N \) to match the number of kinematic constraints on the particles yields

\[
s_c \equiv (3-n_c)z_c/2 \geq 6,
\]

where we have defined the staticity index \( s_c \). The equality corresponds to isostaticity. By analogy to the system in Ref. 22, the response of “hyperstatic” piles with \( s_c > 6 \) to external forces cannot be determined without considering the history of grain contacts.

Figure 4 depicts \( s_c \) as a function of \( \theta \). As expected, \( s_c < 6 \) for all flowing piles, though it increases with decreasing \( \theta \). However, it appears that a finite jump of \( s_c \) at \( \theta_r \) leaves the static pile significantly hyperstatic. Note however that the point denoted by \( * \) in Fig. 4 is for a system where \( k_n = 2 \cdot 10^7 \text{mg/d} \), indicating that grain hardness is a relevant parameter in determining \( s_c \) and \( z_c \).
What do these observations teach us about the nature of the “jamming” transition of the granular medium? Our earlier work showed that granular flows obey a local rheology independent of the history of loading \[10,11\]. Also, static piles are known to generally be able to support a range of external stresses without any macroscopic rearrangement. So, how was the original stress state and associated configuration of grains in this static pile determined? One possible answer is that this state was determined by the local loading conditions at the instant the flow ceased. This resolution is akin to ideas discussed in the fixed principal axes (FPA) model \[4\], except that the stress state of the static pile, including principal stress axes, do change subsequent to flow arrest (which is manifested as burial in the FPA model) as a function of external loading, due to contact elasticity of grains.

We have observed analogies between jamming of granular media and the glass transition. A plateau in the force distributions appears at small forces once the system ceases to flow, as observed in numerical studies of liquids at the glass transition \[8\]. Also, more locally ordered structures appear as the system compact. However, the most significant effect is the transition from a flowing plastic system with a local rheology to a static system that may preserve the fingerprint of the stress state at the instant of jamming, which makes this transition similar to a glass transition, in that glasses also have an ability to be pre-stressed. Finally, we note that we have performed a similar study with Hookean spheres, with essentially the same results.

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