Transitions in the response of a granular layer

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Abstract. The response of two dimensional granular slabs to vertical localized loads has been studied using MD simulations, and characterized by a function that measures the departure of the response from linearity. This function is usually continuously increasing, but in some cases it experiences distinct jumps. A study of the corresponding force chain network reveals that these jumps are associated with the establishment or loss of “critical” contacts to which the system is highly sensitive.

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INTRODUCTION

The properties of densely packed granular materials in both the static and flowing states are of much current interest [1, 2], mostly due to the unusual properties often exhibited by these systems and their industrial and environmental importance. Some successful phenomenologies have been developed in the realm of dense granular flows [3]. The transition between the static state and the flowing state of a granular system is often associated with the “jamming transition”; much effort has been directed towards the elucidation of the nature of this transition [4, 5, 6, 7]. The jamming transition can be approached from the flowing side or the static side. Here we focus on the latter but do not study the transition as such. Prior to reaching the putative jamming point a solid granular system must experience changes induced by external forces; these can cause the necessary plastic events that precede the transition to flow. It is the goal of this paper to shed some light on this process.

A rather well researched granular system is that of a vertical, 2D or 3D slab, subject to a point-force at its top. When this force is sufficiently small the response of the slab is elastic, as revealed in the study of Lennard-Jones glasses [8] and theoretical and experimental studies of granular slabs [9, 10, 11, 12, 13, 14, 15]. Sufficiently large forces induce rearrangements of the packing [16] and departures from elasticity [17, 18, 19]. In Lennard-Jones glasses, these rearrangements are associated with quadrupolar localized events and shear bands [20]. In granular systems, sufficiently large forces cause significant amounts of sliding contacts, the establishment of new contacts and the severing of others. Below we demonstrate that the departure of the response of a granular slab from linearity (hence, linear elasticity) proceeds smoothly as the external force is increased but at times it exhibits significant jumps which are results of changes in some critical contacts, often single contacts. Clearly the sensitivity of the system’s response to such singular events is stronger the smaller the system and therefore, as shown in [18], these rare but strong jumps are consequential in not-too-large systems on a global scale but only locally (near the point of application of the force) in sufficiently large systems.

NUMERICAL METHOD AND ANALYSIS

The Cundall and Strack model [21, 22] for the particle interactions is employed. Damping is implemented along the normal direction only and set to its critical value. Coulomb friction is accounted for. Our molecular dynamics (MD) code employs a third order predictor-corrector integration scheme for solving Newton’s equations of motion with the above model interactions. The studied systems are two-dimensional vertical layers typically comprising a few thousand polydisperse grains. First, the system is prepared by a sequential deposition of grains and run till static equilibrium is obtained, as judged by a rather stringent set of criteria [13, 19]. Next,
FIGURE 1. The measure, $\Delta$, for a single realization of the slab. $Z$ is the mean height of the externally forced particles. Details on the configurations denoted by A, B and C are shown in Fig. 2. The inset show the averaged stress profile for the entire layer. Though some individual response profiles are double peaked, the mean averaged response is always single peaked.

a grain close to the surface is selected and a downward pointing vertical force, whose norm is slowly increased to a chosen final value, $F$, is applied to it. The simulation is then continued until a new static state is reached. The response of the layer is defined as the stress field difference between the loaded state and the unloaded one. The stress response function is computed from the contact forces and grain positions, using an exact coarse graining method [23, 24]. The result depends weakly on the choice of a coarse graining function, $\Phi$, and coarse graining scale, $W$. Within the range $d < W < 10d$ ($d$ is the mean grain diameter), the stress exhibits a plateau whose width increases upon ensemble averaging [14]. Here, we use $W \approx 6d$ and focus on the vertical component of the response at the bottom of the layer, $\sigma_{zz}$. Examples of the variation of $\sigma_{zz}$ with the horizontal distance to the point of application of the force, $x$, are shown in the inset of Fig. 1. These profiles have been obtained for different values of the force, and normalized by $F$ in order to show the linearity of the response.

We define a measure of the deviation of the response from linearity as follows:

$$\Delta = \sqrt{\frac{1}{2L} \sum_{i} \left( \frac{\vec{F}_i}{F} - \frac{\vec{F}_0}{F_0} \right)^2},$$

where the subscript $i$ denotes the $2L$ fixed grains at the bottom of the layer. $F_0 = 0.125 (\langle m \rangle g)$ is a reference small overload force, $\vec{F}_i$ and $\vec{F}_0$ are the forces exerted on grain $i$ in the considered and reference states, respectively. Clearly, $\Delta$ is the RMS of the normalized difference between the response profiles. Obviously, $\Delta \to 0$ indicates that the response is linear (as expected for small loads).

The dependence of $\Delta$ on $F$, for nearly four decades of the latter ($0.125 < \frac{F}{\langle m \rangle g} < 400$), is displayed in figure 1. One can see a low plateau at small and moderate values of $F$, corresponding to the linear (elastic) regime, followed by an increase of $\Delta$ at larger forces.

Figure 2 depicts the force contact network corresponding to selected points in Fig. 1: the grains are shown as circles and (response) contact forces are denoted by lines that connect the grain centers and whose widths indicate the relative strength of the forces. Only forces larger than 2% of the external load are shown. Red/black lines indicate that the contact force is larger/smaller than in the reference state. A grey rectangle is drawn just above the loaded grain; its size is proportional to the magnitude of the external force. Blue discs represent pairs of grains that established contact and red ones indicate severing of the corresponding contact with respect to the reference state. The results presented below have been obtained...
Figure 3. The measure, \( \Delta \), for a single realization that exhibits a noticeable discontinuity that corresponds to a structural rearrangement in the layer structure, see Fig. 4. The inset corresponds to a small force range around the discontinuity (with a step of 0.01 \(< m > g\) to capture the jump at 16.49 \((m\ g)\).

from the analysis of 5 slabs comprising 3721 grains each. A total of 121 points of application of the external force and 24 different values of the magnitude of this force have been studied.

RESULTS AND DISCUSSION

The increase of the measure, \( \Delta \), with \( F \) can be continuous and monotonic, like in Fig. 1, and is associated with a slow and continuous widening of the stress response profiles: this is the generic case. It can also exhibit abrupt changes or “jumps”, as illustrated in Figs. 3 and 5. These strong discontinuities correspond to significant changes in the stress response functions: in Fig. 4 one observes that a double-peaked profile changes into a single-peaked one whereas in Fig. 6, a reverse transition occurs. There are also smaller discontinuities that do not seem to have a prominent effect on the stress response profiles.

At the microscopic level, two kinds of rearrangements can arise. A contact can slide when the tangential to normal force ratio exceeds the Coulomb criterion. Contacts can also open or close. These events are often highly localized but at times they affect many of their neighbors. Rearrangements that take place far from the point of application of the external force do not have much of an effect on the value of \( \Delta \) or the stress response profile whereas rearrangements that occur in the vicinity of the point of application of the external force and in particular those that affect strong force chains that emanate from this point induce significant changes in the contact force distribution and the corresponding stress response profiles.

Goldenberg and Goldhirsch [17, 18] discovered that the stress response functions for forced 2D slabs undergo a transition from a single peaked to a double peaked shape as the force is increased. The latter case was identified as resulting from major rearrangements (mostly,
FIGURE 5. Yet another sharp transition as a function of the external force and a corresponding zoom of the neighborhood of the transition. Here the value of the force at the discontinuity is $F = 9.77 \langle m \rangle g$. The notation is as in Fig. 3.

The contact force network that corresponds to Fig. 5. The stress response function shown in the insets exhibits a transition that is the reverse of the one shown in Fig. 4.

the severing of contacts) that (nearly) reach the bottom of the slab and as such are finite size effects (for a very large system the same force does not lead to such a global rearrangement). The systems studied here are characterized by a stronger polydispersity and disorder than theirs and are therefore richer in the types of behavior they exhibit. However, the basic conclusion concerning the fact that the observed changes in the stress response function qualify as finite size effects carries over to the cases considered here.

Interestingly, stress jumps have also been observed and carefully characterized by Combe and Roux [25] in numerical biaxial tests performed on samples comprising poly-disperse, rigid and frictionless grains. Such systems generically form isostatic packings, i.e. they are at the jamming transition - the intergranular contact network is just sufficient to support an external loading [26, 27] and exhibit ‘soft modes’ by which the system can rearrange at vanishing energy cost [27, 28]. Combe and Roux found that the stress-strain curves corresponding to the systems they studied consist of successions of steps that persist even in the limit of large systems - the axial strain dependence on deviatoric stress is a Lévy stochastic process. Their findings may not carry over to systems of frictional grains [29].

While the study presented here is still a long way from making contact with the properties of the jamming transition, we believe it presents some properties that may hold even near that transition and help further elucidate its nature. Other interesting systems to be studied using similar methods would be inclined slabs just below the angle of repose. Further studies that distinguish between finite size effects and properties that survive system-size upscaling, are in order as well.

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