On the reversibility of granular rotations and translations

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We analyze reversibility of both displacements and rotations of spherical grains in three-dimensional compression experiments. Using transparent acrylic beads with cylindrical holes and index matching techniques, we are not only capable of tracking displacements but also, for the first time, analyze reversibility of rotations. We observe that for moderate compression amplitudes, up to one bead diameter, the translational displacements of the beads after each cycle become mostly reversible after an initial transient. By contrast, granular rotations are largely irreversible. We find a weak correlation between translational and rotational displacements, indicating that rotational reversibility depends on more subtle changes in contact distributions and contact forces between grains compared with displacement reversibility.

I. INTRODUCTION

Flows of granular matter are an important subject of study in many fields, including geology (where they are relevant for avalanches and earthquakes), engineering (where they play a role in industrial processes and construction), and astronomy (where they affect the formation of asteroids and planets). In these contexts, it is particularly important to understand how the granular material transitions from a jammed state to a state of flow with irreversible rearrangements. A common driver of granular flow are cyclic perturbations, which can be caused by a wide range of driving forces, such as vibrating apparatus (construction), periodic loads (roads and rails), earthquakes, cyclic gravitational fields (tidal forces), or thermal expansion and contraction due to day/night temperature variations (on planets and asteroids). Beside the question of flows, the cycling compression or shearing of the granular system can change the properties of the packing, leading to compaction[1] and ultimately crystallization in some cases [2, 3].

Most past numerical and experimental work in this area has concentrated on the translational motion of particles and the associated force fields. However, granular systems are frictional and often aspherical, which implies the presence of rotations of the grains. Rotations and torques can play an important role in mesoscopic granular motions, as has been shown in two-dimensional investigations[4]. Thus bulk granular mechanics is affected by both force networks and torques, though rotations and torques are often ignored, with the notable exception of the Cosserat continuum elastic models [5].

Furthermore, rotations are likely more important in "real" three-dimensional systems of spherical particles than in two-dimensional model systems. In a three-dimensional frictional system (i.e., a system where rotations matter), the number of constraints increases by 3 to a total of 6, as compared to a non frictional system, while it only increases from 2 to 3 in two dimensions. Thus frictional, rotating systems in three dimensions could become isostatic with only four contacts, long before the jamming point at 6 contacts per particle[1]. A typical frictional packing is thus overconstrained due to the frictional forces. The distribution of forces, between normal and frictional, is then dependent on the history of contacts[6], i.e., the method of preparation of the system. Periodic compression of a frictional system will alter the contact distribution and could lead to a different state of the system, called a random loose packing, in contrast to the random close packing with six contacts per particle that we would find for a frictionless system. Thus understanding rotations is important to elucidate the nature of different jammed states of frictional spherical (or aspherical) particles as well as their transition to flow.

Despite the importance of rotations for granular systems, only a handful of experimental investigations have studied them [7, 8], especially in three dimensions[9–12]. In this study of reversibility we build on our first experimental measurements of particle-scale rotations in a three-dimensional granular flow [13], and systematically measure both rotations and translations together under cyclic forcing. To focus our investigation on irreversibilities associated with rotational motion, we study small enough driving amplitudes so that the translational motion of the translational motion of the system is reversible. We had previously shown that in this small forcing regime, convective flows and segregation—two hallmarks of bulk granular flow—are also suppressed[14].

II. EXPERIMENTAL SETUP

The experimental setup, sketched in figure 1(a), is composed of a container with transparent polycarbonate walls filled with transparent acrylic beads. The container is 15.24 cm wide (y direction) and approximately 15 cm long (x direction). The back aluminum wall is displaced by a motor to compress the whole system. The amplitude of compression was varied between 0.5% and 2.5% of the container length [15]. At this amplitude, our experimen-
tual system is still below the convection regime, which will invariably appear at higher amplitudes [16]. The compression speed was 0.05 mm s\(^{-1}\) for all amplitudes, i.e. a constant shear rate. We verified that this speed is slow enough to expect granular rearrangements that resemble dry systems [17]. All the experiments contained between 500 and 1000 cycles of compression, with between 4 and 16 three-dimensional images captured during each cycle. All figures in the manuscript are presented for the case of 2.5\% compression, unless noted otherwise.

The container is filled with 20,000 transparent acrylic beads of radius \( R = 2.5\text{ mm} \), forming a height (z direction) of approximately twenty layers. Each bead has a 1.4 mm diameter cylindrical cavity running through it, allowing us to detect the orientation of the bead. A 1.5 kg transparent acrylic weight is placed on the beads to maintain a constant pressure. The beads and the weight are submerged in an index-matched solution of Triton X-100, which additionally includes a fluorescent Nile blue dye as well as 0.05 \% of hydrochloric acid (38 \% concentration) for effective dilution of the dye [18]. The whole system is illuminated with two 660 nm [19] scanning sheet lasers from both sides of the container.

We should note that a single hole in the grains does not allow us to detect rotations when the axis of rotations is along the hole of the bead. Only rotation components perpendicular to the hole can be resolved. Thus, we focus on small amplitudes where particles retain their translational mobility, only the rotational mobility is along the hole of the bead. Only rotation components perpendicular to the hole can be resolved. Thus, only translation or its correlation with other quantities. Given the statistical analysis of amplitudes of rotations, not taking into account such information as the axis of rotation and all the particles whose motion during the compression cycle is less than the standard error.

III. TRANSLATIONAL AND ROTATIONAL DISPLACEMENTS

We denote by \( \vec{x}_i^T \) the position of particle \( i \) at the temporal position \( T \) (one of A–E) in the cycle and by \( \vec{q}_i^T \) its orientation expressed as a unit vector. We introduce the relative (as compared to the beginning of the cycle) displacements of particles at time \( T \): the translational \( \mu_i^T = \| \vec{x}_i^T - \vec{x}_i^A \| \) and the rotational \( \theta_i^T = \sin^{-1}(\| \vec{q}_i^T \times \vec{q}_i^A \|) \), as well as their averages: \( \langle \mu^T \rangle = \frac{1}{N} \sum_{i=1}^{N} \mu_i^T \) and \( \langle \theta^T \rangle = \frac{1}{N} \sum_{i=1}^{N} \theta_i^T \).

Figure 1 d) shows a snapshot of typical translational displacements of the particles at time \( C \). The gradient angle matches the symmetry of the system, with a compressing right wall and movable top wall kept at constant pressure. In contrast, the rotations do not present any apparent shear zones, with a larger concentration of rotations near the bottom of the cell, suggesting an absence of direct correlation between translations and rotations. This is corroborated by statistical analysis as presented below.

We now turn to the study of the reversibility of granular displacements. Note that due to the nature of our experiments, a small but measurable compaction (following a power law) is found as expected [20] in our system. While the particle positions are not perfectly reversible, we focus on small amplitudes where particles retain their neighbors, and where (as shown in [14]) convection and segregation are suppressed. In this regime, where the position of most particles with respect to their neighbors is reversible, we investigate rotations, as well as their evolution with cycle number.

To examine the irreversibility of the granular motion we can study the translational and rotational displacements of particles at the end of the cycle: \( \mu_i^E \) and \( \theta_i^E \). As can be seen in scatter plots of translations and rotations (figure 2), comparing the displacements of each particle at time \( C \) to the displacements at time \( E \), translations
are reversible as expected, while rotations are mostly irreversible. For the translations, almost all of the displacement is reverted at the end of the cycle in contrast to the rotations for which a lot of particles do not return to their initial orientation.

To obtain a better statistical understanding of the phenomena, we compare the average of end-of-cycle displacement of the particles to that of their mid-cycle displacement. Figure 3 shows the expected end-of-cycle displacements $\mu_E$ and $\theta_E$ for given values of mid-cycle displacements $\mu_C$ and $\theta_C$. These are well characterized by power-law behaviors with approximate exponents of $\approx 0.35$ for translations and $\approx 0.43$ for rotations at moderate displacements. As seen in the figure, these exponents do not depend on the amplitude of compression of our system, indicating a universal behavior for the amplitudes we investigated. At very large values of translation displacement the exponent seems to increase. This probably correspond to a transition to diffusive behaviour when beads move so much that they can escape their “cage”. Both the translational and rotational exponents are smaller than 1, which implies that the relative reversibility improves for bigger displacements. We introduce relative irreversibility parameters $I_{\mu,i} = \mu_E^i / \mu_C^i$ for translations and $I_{\theta,i} = \theta_E^i / \theta_C^i$ for rotations which plotted against the mid-cycle displacements $\mu_C$ and $\theta_C$ give the expected mid-cycle exponents of $\approx -0.8$ and $\approx -0.6$ (figure available in supplemental part III).

We have studied the correlation between translations and rotations and have found that the expected middle or end-of-cycle rotational displacements $\theta^{C,E}$ and translational displacements $\mu^{C,E}$ are very weakly correlated (figures available in supplemental part IV). This result
is in contrast to the case of ellipsoidal particles, where a strong correlation between rotations and translations was experimentally found [12]. The difference can be explained by the fact that for ellipsoidal particles rotations imply a change in the effective volume occupied by the particles and thus can simply couple to translations of surrounding particles.

Beyond the reversibility to its initial position and orientation, we investigate the reversibility of the whole particle trajectory, both in terms of translation and rotation. We plot the displacements of particles during a cycle of compression averaged over similar values of mid-cycle displacements (Fig. 4). These results are based on the actual motion of the moving wall, corrected for slight backlash present in our experimental system.

Figure 4 highlights the difference between the behavior of granular translations and rotations. Translations are very reversible, with beads following much of the same path during compression and dilation, especially at high values of the wall displacement. On the other hand, the rotation trajectories are much less so; the dilation path, which begins at maximum wall displacement and goes back to zero wall displacement, diverges almost immediately from the compression path. In other words, in contrast to the translations, the forward and backward paths for rotations differ significantly even close to point of wall reversal (maximum wall displacement). The reversibility of both translations and rotations improves after many cycles as compared with the beginning of the experiment (figures in supplemental part V), suggesting that, after an initial transient period, the system self-organizes into a more reversible configuration.

IV. CONTACT DYNAMICS

For particles to revert back to their original positions relative to their neighbors without reversal of orientations requires some change in frictional contacts. To study the contacts dynamics, we define particles that are within a cutoff distance $r_c$ of each other as being likely in con-
tact. To capture all likely contacts we chose $r_c$ as the
distance within which particles have on average 6 con-
tacts per particle, significantly above the isostatic limit
for frictional particles[21]. We have verified that varying
$r_c$, such that the mean number of contacts per particle is
between 4, the isostatic limit for frictional particles, and
6, the jamming point, does not change the quantitative
results presented here.

We define $\chi^T_1$ as the total number of contacts of an
individual particle at time $T$. While the translational
displacement are weakly correlated with the number of
contacts a particle have at the begining of the cycle, the
rotational displacement are strongly dependent on this
quantity as shown on Figure 5. Particles with fever con-
tacts tend to have much bigger end of cycle rotations.
This suggests that particles that can rotate more freely, are
less prone to return to their original positions. Note that
in frictional contacts the transition between the “rolling”
and “slipping” phases is hysterical. This means than
even a conservacy of contact points does not guarantee
the reversal of rotational motion. Indeed, while we find
that both translational and rotational irreversibility are
strongly correlated with a gain or loss of a contact (not
shown), translations are more affected.

V. SUMMARY AND CONCLUSIONS

We conducted a novel experiment allowing us to track
translations and rotations of particles in three dimensions
during cycles of uniaxial compression. We found that the
overall reversibility of translations is much higher than
that of rotations. This is explained by the absence of di-
rect correlations between the rotations and translations;
the reversible motion of particles “trapped” in cages[16]
does not imply the reversibility of rotations. Given the
available results of a presence of correlations between
translations and rotations for ellipsoid particles[12], a
larger correlation between translations and rotations may
be observed for larger friction and different frictional
properties of the particles. In our system, the non-
reversibility of rotations is a possible mechanism for the
system to maintain a memory of cycling, even under
small forcing conditions that do not imprint a memory in
“bulk” indicators of prior forcing (segregation, comp-
paction).

Even though most particles retain their neighbors in
our experiment, their contact-point dynamics follows a
more hysteretic path and rotational motion is not re-
versible. It is highly probable that the irreversibility of
rotations is also reflected in a parameter which we can-
not track in our experiments: the force distributions. To
elucidate this hypothesis, further work is needed to track
the rotations and the forces on the particles at the same
time, either through simulations or different experimen-
tal methods[22].

An important aspect of granular flow is the vector of
rotation compared to the direction of shear/compression.
It has been predicted[23] that particles will rotate per-
dicular to the shearing motion. However, to verify
this hypothesis experimentally, we need to access all three
degrees of rotations, which will be the subject of our fu-
ture work.

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Supplemental material for

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I. CONTACTS BETWEEN PARTICLES

Our particles possess a hole that allows to track rotations. It is justified to question if other particles will be inclined to “fall” into this holes and if they do, whether it will affect the translational and rotational motion of the particles. Let us call $\alpha$ the angular opening of the hole as shown on figure 1 a). A straightforward calculation will give

$$\alpha = 2 \sin^{-1}\left(\frac{d}{D}\right)$$

where $D = 5\, mm$ is the diameter of the bead and $d = 1.4\, mm$ is the diameter of the hole. Given an axis normal to the surface of the bead, the probability that a contact point will be located within an angle $\beta$ of this axis is given by the surface area located within this angle. We can then easily show that this probability is given by

$$P(\beta) = 1 - \cos(\beta) = 1 - \sqrt{1 - \sin^2(\beta)}$$

If we define a contact through a hole as any contact whose contact point is located within an angle $\alpha/2$ of the hole axis, then the theoretical probability of contacting through the hole is given by

$$P\left(\frac{\alpha}{2}\right) = 1 - \sqrt{1 - \left(\frac{d}{D}\right)^2} = 4\%$$

To check this prediction we compute the probability of a contact happening at a particular angle from the axis from our experimental data. To detect a contact we consider all beads located within a cutoff distance $r_c$ as being in contact. The value of $r_c$ is determined in the same way as outlined in the part IV of the main article. We compute the probability this probability both at the beginning and the end of the experiment. The result is presented on figure 1 b). We can see that the actual probability of contacting through a hole is higher than the theoretically predicted value indicating that indeed the particles tend to “fall” inside the hole. The experimental cumulative probability of contacting through the hole is $\approx 12\%$. Note that the increased probability of a contact happening through the hole, also increase the
Figure 1. a) Sketch of the contact through a hole. Note that an increase in the probability of contacting through a hole will also increase the probability of a contact happening at 60° from the hole axis. b) Experimental probability of a contact point being at a certain angle to the hole axis. Green dots indicate the beginning of the experiment, yellow dash the end of experiment and black line the theoretical predicted value for an equal probability contact point.

probability of a contact happening at 60° from the hole as explained on figure 1 a). However we can see that the probability of contacting through a hole is unchanged at the beginning of the experiment as well as at the end of the experiment. This means that there is no tendency for the “crystallization” of hole contacts.

We can ask the question if the particle contacting through a hole will see their dynamics impacted as to the particles which do not contact through the hole. For this end we measure the probability of translational and rotational displacements at times $C$ and $E$ as compared to the beginning of the cycle. We measure these quantities separately for particles that do contact through a hole at the beginning of the cycle and particles that do not. The results are presented on figure 2. We can see that translations are unaffected by the type of contact. Only rotations suffer a small decrease in their amplitude while maintaining the overall shape of the distribution. Note that this decrease in rotational mobility emphasis even more our funding on the irreversibility of the rotational dynamics.
Figure 2. Probability of translational (a and b) and rotational (c and d) displacements between the beginning and middle (a and c) and end (b and d) of cycle. Yellow line indicate particles that do not contact through their hole at the beginning of the cycle, while green circles indicate particles that do contact through the hole.

II. SNAPSHOTS OF DISPLACEMENTS

We can compare the snapshots of the amplitude of displacement between the fully compressed state C and the fully decompressed state E. We can see in figure 3 that while most particles go back to their original position under translation, a lot do not under rotation. We also note the absence of any apparent shear bands for the rotations.
Figure 3. Snapshots of translational (a and b) and rotational displacements (c and d) at times C (a and c) and E (b and d). Amplitude in mm. Videos of full compression cycles are available in the supplemental material.

III. IRREVERSIBILITY OF DISPLACEMENTS

In addition to studying the translational and rotational displacements, we can introduce the relative irreversibility parameters $I_{\mu,i} = \mu^E_i / \mu^C_i$ for translations and $I_{\theta,i} = \theta^E_i / \theta^C_i$ for rotations. As seen in figure 4, both of these show decaying power laws as a function of the mid-cycle mobility, with exponents of $\approx -0.8$ and $\approx -0.6$ for translations and rotations respectively.
IV. CORRELATIONS BETWEEN TRANSLATIONS AND ROTATIONS

To investigate the presence of correlations between rotations and translations, we plot averaged values of one against the other in figure 5. While small variations are present they are negligible compared to the decades of variation of mobilities seen in figure 3 of the main article.
Figure 5. (a) Averaged value of rotational displacement binned over values of translational displacement at state C. (b) Averaged value of translational displacement binned over values of rotational displacement at state C. (c) and (d) same as (a) and (b) at state E. All units in mm.

V. CYCLES OF DISPLACEMENT

In addition to plotting the cycles of translational and rotational displacements at the end of the experiments we can plot the same quantities at the beginning of the experiment to compare the change in the irreversibility.
Figure 6. Bead translational (a) and rotational (b) displacement cycles averaged over identical mean mobilities for the first five cycles. Compare with figure 4 in the article where the same quantities are plotted for the last ten cycles of the experiment. The mid-cycle mobility goes from $6 \times 10^{-1} \text{ mm}$ to $3 \text{ mm}$ for translations and from $1 \times 10^{-1} \text{ mm}$ to $3 \text{ mm}$ for rotations. All units in mm.