Study of Quasi Two Dimensional Granular Heaps

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Density distributions in granular heaps have up to now been mostly investigated with the discrete element method (DEM) in two dimensions, as few research groups have the necessary simulation codes for non-spherical particles in three dimensions. The angle of repose of quasi-two dimensional granular heap in three dimensional simulation is higher and therefore more realistic than two dimensional simulations. We investigate the density distribution in a granular heap between walls in relation to the “pressure dip” with a three dimensional DEM simulation with polyhedral particles. We verify the results experimentally with glass beads in a similar configuration. We find consistent density patterns in the experiment and in the simulation.

1. INTRODUCTION

There is generally a problem in granular materials research in relating two-dimensional results (i.e. results with two-dimensional materials, like rods, i.e. Schneebell-Material) with quasi-two-dimensional results (three-dimensional grains between two narrow walls) and fully three dimensional geometries (i.e. unbounded, cone-shaped heaps). For the formation both of actual and quasi-two-dimensional heaps, avalanches would be restricted to go either “to the left” or “to the right”, while on surfaces of conical heaps, continuous direction changes are possible. The heap geometry will also affect the internal dynamics. While for two- and fully three-dimensional heaps the ground would carry the whole weight, quasi-dimensional heaps would act as silos, i.e. a part of the weight of the heap may be carried by the walls, depending on the height of the heap and the narrowness of the wall, due to the Janssen-effect 1).

A massive controversy arose in the granular community about the occurrence of pressure dips (relative minima in the pressure distributions in the center of heaps between larger pressure amplitudes) of granular heaps in the second half of the 1990s, see the literature 2, 3, 4) and references therein. As one of the authors 2) pointed out, mostly papers from powder mechanics (poured from a point source) showed pressure minima, papers from civil engineering (built layer-wise) did not. While arching was discussed as a prime suspect, the identification of the mechanism which causes the arching is still under debate. Savage 3) had pointed out layer-wise in the weight computation of heaps built from point sources. Subsequently Schinner 4) found in two-dimensional simulations pressure minima under cores with higher density for heaps built from point sources, and “flat” pressures under homogeneous dense heaps which had been built layer-wise, which indicated that density inhomogeneities were the cause of “arching” and “pressure minima”. For experiments of quasi-two dimensional heaps of glass beads between parallel walls, Chen et al. 5) found density patterns consistent with the two dimensional polygonal simulations. In this paper, we would like to go as far as possible to show that density inhomogeneities are not just an artifact of two dimensional simulations, but exist also in three dimension, both in simulation and experiment.

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Beyond the geometrical differences, dynamically, there are more rolling degrees of freedom in three dimensions, so the competition between rolling and sliding in the formation of the heap is also different. Therefore, for an understanding of realistic granular heaps between narrow walls, a full three dimensional simulation is necessary, though up to now most of the simulations concerning the density distribution were two dimensional \([5, 6, 7]\) or only for round particles \([8]\).

In this paper, we will study the density distribution of quasi-two-dimensional granular systems both experimentally and numerically. Compared to numerical simulations, experimental studies of density distribution inside granular heaps are of great difficulty or cost. With nuclear magnetic resonance (NMR), Šmid et al.\(^9\) had found elevated densities in the middle of silo fillings from a point-source. Matuttis \(^{10}\) and Chen et al.\(^9\) succeeded to calibrate laser-sensor pairs for production engineering to measure the density distribution of granular heaps constructed from glass beads deposited between two narrow transparent walls. We have improved our optical measurement method \([5, 10]\) to capture the density inhomogeneous inside the heaps (Section 2), while applying our newly developed three-dimensional DEM code with convex polyhedral particles to form a quasi-two dimensional heap and investigate its density distribution and bottom pressure distribution.

![Sketches of the dispersion of a laser beam going through a granular system](image1)

![A laser-sensor pair to measure the strength of the laser beam after dispersion](image2)

**Fig. 1** Sketches of the dispersion of a laser beam going through a granular system

**Fig. 2** A laser-sensor pair to measure the strength of the laser beam after dispersion

### 2. EXPERIMENTAL INVESTIGATION

When a light beam travels through transparent granular particles, the intensity of the beam will decrease due to dispersion (scattering at the particle surfaces away from the initial direction of incidence, Fig. 1). The scattering per covered distance is stronger for more particle surfaces in the optical path, i.e. it increases with density and decreases with the size of the particles. This leads to a characteristic decrease of the light transmissivity which can be formulated like an exponential decay rate \(^{10}\). Thus we apply a laser-sensor pair (Fig. 2) to measure the density distribution in granular-glass-bead heaps with the calibration for densities of a given particle size.

#### 2.1. CALIBRATION

The calibration setup is shown in Fig. 3: A container with adjustable width and fixed length and height (150 mm × 65 mm) is placed in-between of a laser-sensor set (Keyence FU-E11/FS-N11MN) and the measured laser intensity from the sensor can be read from a meter as a quantity ranging from 0 to 9999. For a selected width (e.g. 15 mm), the volume of the container is constant. By filling the container with varying amounts of glass beads and varying the filling method, we could obtain different homogenized packing densities for the granular assembly in the container. For calibration, the container should be filled as even as possible to minimize the density difference among the granular system to be measured. Lower densities can be obtained by filling the container when it
is laid nearly horizontally and then turn it upright while high density by vibration, e.g. tapping the container or shaking it along the z-axis to let the particles compactify to a closer packing. Since the measured intensity decays exponentially with the increase of the width of the container in such systems \(5, 10\), we calibrated the new laser-sensor set only for the granular assembly of 15 mm width. The container is filled with 210 g, 225 g, 240 g, 255 g and 277 g non-spherical glass beads of 2-4 mm length, as shown in Fig. 3. The calibration between the averaged packing density and the readings of the measured laser intensity is shown in Fig. 4. The “error bar” should rather be interpreted as a signature of the inhomogeneous density than actual measurement error. The calibration curve shows the capability of the laser-sensor set to resolve a density difference of about 0.1 g/cm\(^3\) (approximately 5% to 6% with respect to the mean packing density). With least squares fitting of the experiment data, we obtained an exponential relation between the intensity reading \(I_r\) and the packing density \(\rho_p\) as

\[
\log I_r = -3.69\rho_p + 7.14, \tag{1}
\]

where \(\rho_p\) is a dimensionless variable obtained from recalling the filling density with the bulk density of the glass beads, 2.78 g/cm\(^3\). Using Eq. (1), we can then recalculate the average density distribution inside the heap from the intensity data. Due to low transmissivity, measurements can be obtained for heaps which are up to few tens of particles in the width dimension.

![Calibration Setup](image1)

**Fig. 3** Calibration setup and samples of glass beads used for experiment

![Calibration Result](image2)

**Fig. 4** Calibration result: each data point is the average of 80 measurements

### 2.2. HEAP CONSTRUCTION AND DENSITY MEASUREMENT

We used a “X-Z axis linear robot system" \(5, 10\) (IAI ICSCA2-ZICM-A-60-40B-T1-5L-GT, see Fig.5) for the construction of the granular heaps and the density measurement described in the calibration. The robot can move along the x- and the z-axis with constant speed, making the construction and measurement of granular heaps reproducible. To construct a granular heap, we first fill a hopper with glass beads (the same kind as used in calibration) and put its funnel at the bottom of a acrylic container with 15 mm width (and 1200 mm length and 300 mm height); Then we let the robot lift the hopper at a slow speed (see Fig.6, above) while refilling it to keep a steady granular flow pouring down from the hopper. If the hopper is lifted too fast and the glass beads are accelerated, the heap structure would affected by liquidation of regions by particles with high impact velocity. To measure the density distribution inside the heap, we move the laser-sensor set along the route as shown in Fig.6, below; Then the measured signal of the sensor is recorded by a
data acquisition system (Keyence MS2-H50) for the sensor. With the calibrated relation Eq. (1), we can convert the measured intensity data into density distribution. The experiment results are discussed together with the simulation results in Section 4.

3. SIMULATION

3.1. MODELING OF PARTICLES

Many DEM simulations model particles as two dimensional round discs since Cundall and Strack first introduced DEM to granular media research.\textsuperscript{11} For discs, the contact problem in two dimensions is reduced to a one-dimensional distance calculation. Nevertheless, simulations of discs are unreliable for dense configurations where the competition between rolling and sliding determines the dynamics of the system, e.g. granular heap formation, since the effects of particles elongation and surface roughness (corners) cannot be modeled. Simulations of polygonal shape particles showed that the effect of the particle geometry on macroscopic properties like stress strain relation\textsuperscript{12} and sound velocity\textsuperscript{13} is significant.

To improve the verisimilitude beyond polygonal particles, we recently introduced a full three dimensional simulation method which models granular particles of polyhedral shape (see Fig. 18 in the Appendix). In this paper we use polyhedral particles to construct quasi-two dimensional granular heaps. The vertices of a particle are chosen on the convex hull of an ellipsoid with given half radii and the faces of a particle are triangles or divided into triangles for computational simplicity. Fig. 7 shows the particle shapes used in our simulation, the sizes are rescaled for better visibility, a 400 mm $\times$ 150 mm $\times$ 20 mm container, a hopper with funnel of an inner radius of 9.5 mm and a sample granular particle of 12 vertices choosing from the surface of an ellipsoid of radii as 2 mm, 1.6 mm and 1.6 mm. A certain randomness is introduced in the coordinates of the vertices of each particle while the same 12-vertex-20-face geometry structure and edge connectivity is kept. A snapshot of the centers of mass of the particles from the simulation is shown in Fig. 8 from which we see that the particles fall down from the hopper and pile up inside the container. The detailed outlines of particles are simplified as dots in Fig. 8. Since the size of the particles is so small comparing to the whole heap, the outlines would become illegible.
3.2. EQUATION OF MOTION

The movements of granular particles are decomposed according to König’s theorem \(^{15}\) as translational movements of the centers of mass and rotational movements around the centers of mass. For a granular system of \(n\) particles in three dimension, Newton’s equation of motion for the translational movement is

\[ M \ddot{X} = F, \]

where \(M\) is a \(3n \times 3n\) mass matrix, \(X\) is a vector of the \(3n\) coordinate variables and \(F\) is the external force vector of \(3n\) components. The external force on particle \(i\) is the sum of the gravitational force \(G_i\) and the contact force \(f_c\),

\[ f_i = G_i + \sum_{j=1}^{l} f_{cj}, \]

where \(l\) is the number of contacts the particle involves to and \(f_{cj}\) is the contact force from the \(j\)-th contact. The contact force \(f_c\) consists of the normal and the tangential components. The elastic force in the normal direction is determined by the overlap geometry \(^{14}\) (see Appendix A) and the friction in the tangential direction is the generalization of the two dimensional Cundall-Strack model \(^{11}\) in three dimensions (see Appendix B).

For the rotational degrees of freedom, we need to solve Euler’s equation of motion

\[ \dot{L} = \tau, \]

in which \(L\) is the angular momentum and \(\tau\) is the toque introduced by contact force. Substituting \(L = I\omega\) into Eq. (4) gives

\[ I\ddot{\omega} + I\dot{\omega} = \tau, \]

where \(I\) is the moment of inertia and \(\omega\) the angular velocity. For numerical stability, instead of Euler angles, we choose unit quaternions \((q = [s, (x, y, z)], \quad ||q|| = \sqrt{s^2 + x^2 + y^2 + z^2} = 1)\) and their time derivatives to represent orientations and rotational degrees of freedom of particles. Derived from
Eq. (4) and Eq. (5), the second time derivative of the unit quaternion \( q \) is

\[
\ddot{q} = \frac{1}{2}(\dot{\omega}q + q\dot{\omega}),
\]

(6)

with the auxiliary equations

\[
\begin{align*}
\omega & = 2\dot{q}q^*, \\
\dot{\omega} & = I^{-1}(L \times \omega + \tau), \\
L & = I\omega, \\
I & = RI_{\text{body}}R^T, \\
I^{-1} & = RI_{\text{body}}^{-1}R^T,
\end{align*}
\]

in which \( q^* = [s, -(x, y, z)] \) is the conjugate of \( q \), \( I_{\text{body}} \) the moment of inertia in the body-fixed system and \( R \) the rotation matrix and its transpose \( R^T \). The rotation matrix \( R \) which performs the same rotation as the quaternion \( q \) is given by

\[
R = \begin{bmatrix}
1 - 2(y^2 + z^2) & 2(xy - sz) & 2(xz + sy) \\
2(xy + sz) & 1 - 2(x^2 + z^2) & 2(yz - sx) \\
2(xz - sy) & 2(yz + sx) & 1 - 2(x^2 + y^2)
\end{bmatrix}.
\]

One thing worth mentioning here is the treatment of the torque \( \tau \) as it's side effects for the stability of the simulation of granular system are not as obvious as for the forces. Since granular systems are highly dissipative, various kinds of damping together with friction are introduced when modeling the contact forces. They usually damp out translational degrees of freedom effectively. In two dimensions, friction in tangential direction not only serves as an resistance for the translational degrees of freedom, but also helps to impede the rotational degree of freedom: since there is only one rotation axis with two possible directions and the torque caused by friction would either in or against rotation. In three dimensions, there are infinite possible rotation axes, forces which damp cut linear motion can contribute to torques which accumulate to very high speeds if no countermeasures are taken. To simplify the analysis, we assume that the moment of inertia of a particle is \( l = mr^2 \), where \( r \) is half of the typical length of the particle. Since both the linear acceleration \( \dot{\mathbf{v}} = \mathbf{f}_c/m \) and the angular acceleration \( \ddot{\omega} \propto \mathbf{f}_c/(mr^2) \) are caused by the contact force \( \mathbf{f}_c \), we can obtain the relation \( \ddot{\omega} \propto \dot{\mathbf{v}}/r \). For particles with typical length in the millimeter range, e.g. \( r \approx 0.002 \text{ m} \) in our simulation, the relation becomes \( \ddot{\omega} \propto 500 \dot{\mathbf{v}} \) (all variables in SI unit). During a time interval \( \Delta t \), the angular velocity increment \( \Delta \omega \) is hundreds of times larger than the velocity increment \( \Delta \mathbf{v} \) for the same contact force \( \mathbf{f}_c \). This simple arithmetic shows how large the rotational degrees of freedom may be accumulated during the formation of three dimensional granular heaps of small particles e.g. of typical length in millimeter or even centimeter range. Therefore the proper treatment of the damping for rotational degrees of freedom is also indispensable for three dimensional simulations of granular systems. In this paper, we applied a viscous-like damping for the rotational degrees of freedom, then the total torque a particle subjected to is

\[
\tau = -b \omega + \sum_{j=1}^{l} \tau_{c_j},
\]

(7)

where \( b \) is a friction constant with unit as \([\text{kg} \cdot \text{m}^2/\text{s}]\), \( \tau_{c_j} \) the torque caused by the contact forces of the \( j \)-th contact and \( l \) the total number of contacts the particle involves to. Currently this damping scheme damps out rotational degrees of freedom effectively, in future more attentions should be paid to model the pivoting friction. The exact treatment of friction \(^{16}\) will resolve this issue for good, but the implications for the performance of these algorithms which need the solution of a linear system
in which all contacts enter are not yet clear. As long as we have to work with phenomenological friction models (see the Appendix for the details of implementation) which deal with single contacts and do not take the many particle configuration into account, introducing appropriate damping terms is unavoidable.

3.3. INTEGRATION: BACKWARD DIFFERENCE FORMULA

As numerical approximation for the equations of motion (Eq. (2) and Eq. (6)), the backward difference formula (also called “Gear Predictor Corrector” 17, 18) of second order is used. Its advantage is that it is able to neglect small oscillations in the solution and able to approximate the solutions of some differential equations with transcendental solution with arbitrary large timestep. Moreover, it is an implicit method which does not need a matrix inversion or a solution of a non-linear system of equations if the predictor-corrector formulation is used. With the predictor-corrector formulation, we can solve Eq. (2) and Eq. (6) directly as second order differential equation. To integrate Eq. (6), the predicted values at time $t + \delta t$ for $q$ and its scaled time derivatives $q_1 = \delta t (dq/dt)$ and $q_2 = \frac{1}{2} \delta t^2 (d^2 q/dt^2)$ are

$$
q_0^p(t + \delta t) = q_0(t) + q_1(t) + q_2(t), \\
q_1^p(t + \delta t) = q_1(t) + 2q_2(t), \\
q_2^p(t + \delta t) = q_2(t).
$$

The predicted values of $q$ (and the position vector $X$) are used to update the orientations (positions) of the particles. The torques (forces) are then computed based on the predicted orientations (and positions). The corrector takes the form:

$$
q_0^c(t + \delta t) = q_0^p(t + \delta t) + c_0 \Delta q, \\
q_1^c(t + \delta t) = q_1^p(t + \delta t) + c_1 \Delta q, \\
q_2^c(t + \delta t) = q_2^p(t + \delta t) + c_2 \Delta q,
$$

where $c_0 = 0$, $c_1 = 1$, $c_2 = 1$ are the coefficients of the corrector and $\Delta q = q_2^p - q_2^p$ is the difference between the computed value from the equation of motion ($\dot{q}$ from Eq. (6)) rescaled by a factor $\frac{1}{2} \delta t^2$ and the predicted value $q_2^p$. The position vector $X$ of Eq. (2) is corrected in a similar way. Coefficients for higher order correctors can be found in Gear’s book 17).

While the importance of the normalization of quaternion $q$ to keep its length as unit is stressed by Allen & Tildesley 18, we found that the $\dot{q}$ should also fulfill the constraint

$$
\omega = 2 \dot{q} q^*,
$$

in which $\dot{q} = [s_q, (x_q, y_q, z_q)]$ and $q^* = [s_q, -(x_q, y_q, z_q)]$. Since $\omega$ is a pure vector, the scalar part of the quaternion multiplication $\dot{q} q^*$ at the right of the above equation should be zero:

$$
s_q s_q + x_q x_q + y_q y_q + z_q z_q = 0.
$$

Eq. (11) indicates that the two four-dimensional vectors $(s_q, x_q, y_q, z_q)$ and $(s_q, x_q, y_q, z_q)$ are orthogonal. Thus, at each integration time-step, after normalizing the quaternion, we also need to project $\dot{q}$ onto $\dot{q}$ and take only the component which is orthogonal to $\dot{q}$.

3.4. DENSITY COMPUTATION

There are several ways to define average densities of continuous volumes of granular particles, depending on whether the control volume is defined with or without respect of the particles, and whether only the centers of mass or the explicit volume is taken in account, see Fig. 9 for a two-
Fig. 9 Three density homogenization methods: In black the grains volumes which are counted while the dotted line indicates the $V_c$ used at the given cell.

Fig. 10 Moving cell homogenization scheme: each cell has a neighbor cell with certain overlap along the length direction.

dimensional sketch. In the same way we define the homogenized granular density in three dimensions for a cubic cell as the ratio of the volume occupied by the polyhedral particles $V_i$ inside and the volume of the cell $V_c$ itself:

$$\rho_h = \frac{V_1 + V_2 + \cdots + V_n}{V_c}. \tag{12}$$

We have three obvious possible selections for the $V_i$ and the $V_c$: The simplest way is to choose the volumes of all the particles which have their center of mass in the cell $V_c$ (Fig. 9 left); Adding the volume of the polyhedra which extend beyond the cell $V_c$ to the cell $V_c$ (Fig. 9 middle) is another choice; For our measurement we chose only the volume inside the cell $V_c$ (Fig. 9 right) which gives the most accurate result though it is most time consuming. For our “quasi-two-dimensional” heaps, the density distribution is averaged along the width direction. Along the length direction, a moving cell homogenization scheme (Fig. 10) was used to improve the resolution for a given cell length.

4. RESULTS AND DISCUSSION

4.1. EXPERIMENTAL RESULTS

The angles of repose from the experiment are shown in Fig. 11. The upper heap with a larger angle of repose in Fig. 11 is the result of a low lifting velocity ($2 \text{ mm/s}$) of the hopper with refilling of particles to keep a continuous flow of particles, while the lower one with a quite small angle of repose is caused by the high impact velocities of particles accelerated by a relatively high lifting velocity ($8 \text{ mm/s}$) and the intermittent flow of particles caused by clogging in the hopper. For proper measurements of density distributions in heaps, we need a certain height to keep the quasi-two dimensional structure. Thus, heaps should be built with small inflow velocities, while high inflow velocities decrease the angle of repose and are probably not relevant for the discussion of the pressure dip.

The density measurement in the experiment is averaged every $8 \text{ mm}$ along x-axis and $11 \text{ mm}$ along y-axis. The density results from the experiments for lifting velocities $1 \text{ mm/s}$, $3 \text{ mm/s}$ and $5 \text{ mm/s}$ are shown in Fig. 12, Fig. 13 and Fig. 14 respectively. It seems that in the experiment, due to the shear flow of the avalanches, lower densities could be reached than in the calibration, but the maximal densities of the calibration due to tapping and vibrating could not be reached. The experimental data towards the ground (right graphs in Figs. 12-14) show a high density core near the center (middle graphs in Figs. 12-14) of the heap close to volumes with lower densities.
Fig. 12  Experiment for a lifting velocity 1 mm/s: Two dimensional normalized density contour plot (left), average density along the length dimension (middle) and average density along the height dimension (right).

Fig. 13  Experiment for a lifting velocity 3 mm/s: Two dimensional normalized density contour plot (left), average density along the length dimension (middle) and average density along the height dimension (right).

4.2. SIMULATION RESULTS AND COMPARISON WITH THE EXPERIMENT

By implementing the damping for rotational degrees of freedom discussed in Section 3, we could obtain realistic angles of repose for the simulation like the upper heap of Fig.15, while without the damping mechanism, the angles of repose are significantly reduced like for the lower heap of Fig.15. In the simulation, we measure the density distribution of a heap whose angle of repose is higher than the $30^\circ$ obtainable with polyhedrons in two dimensional simulations $^5$ and much larger than simulation with round particles (about $22^\circ$ $^{19}$), if no unphysical tricks like elimination of the rotational degrees of freedom or unphysical large rolling frictions are used). The physical parameters for the simulation are as follows: the Young’s modulus is chosen as $Y = 6.5 \times 10^7$ N/m$^2$, the density as $\rho = 1000$ kg/m$^3$ and the coefficient of friction as $\mu = 0.65$. A fixed timestep of $dt = 6 \times 10^{-6}$ s is used for the time integration and the time span is 12 s. There are 3500 particles in the simulation for the upper heap of Fig.15 and 1800 particles in the lower one. The angle of repose of the former is comparable to the physical experiment and its density distribution is measured.

The density result from the simulation is shown in Fig.16. The density is homogenized in cells of $8 \text{ mm} \times 8 \text{ mm} \times 8 \text{ mm}$ and averaged along the y-axis. When we lift the hopper with funnel (e.g. see Fig.7), the impacting particles vibrate the particle layer below them, which explains the reason of high density in the center. On the other hand, those particles which are not deposited
Fig. 14  Experiment for a lifting velocity 5 mm/s: Two dimensional normalized density contour plot (left), average density along the length dimension (middle) and average density along the height dimension (right).

Fig. 16  Simulation results: Two dimensional normalized density contour plot (left), average density along the length dimension (middle) and average density along the height dimension (right).

in the middle, but which move to the left and right in the shear flow of avalanche or which lead to slippage of particle layers below them create regions of low density. The reduced densities on the ground, away from the center, can be attributed to avalanches which are deposited without much reordering. Compared with the experiment, the simulation result has higher resolution and shows a pattern with less fluctuation: the higher density regions in the middle surrounded by regions with lower density. Also in the simulation, the density increases towards the ground (right graph in Fig. 16) and in the middle (middle graph in Fig. 16). Thus, both the results for the experiment and the simulation show a consistent density distribution pattern of the quasi-two dimensional heaps.

Fig. 17  Simulation results: Pressure on the bottom for the homogenization cell length of 8 mm (left) and the cell length of 12 mm (right).

The pressure distribution in the simulation shows a minimum with different lengths of the sampling cell (Fig. 17), so the correlation of the density maxima with the pressure dip is established also for the three dimensional simulation. Unfortunately, we have up not now not been able to find an affordable experimental device for the experimental measurement. The weight taken by the ground is 85% of the total weight of the heap. As the ratio of the length to height to width of the heap in the simulation is about 140 : 50 : 20, the Janssen-effect is not as marked as it would be for “silo geometries” where the height is considerably larger then the width.
5. SUMMARY AND CONCLUSIONS

For the verification of our three-dimensional simulation with polyhedra, we have calibrated a laser-sensor pair to measure the density distribution of the quasi-two-dimensional heap constructed by depositing glass beads between two narrow acrylic walls. Attention should be paid to the damping of the rotational degrees of freedom in the dynamic simulations of granular systems in three dimensions as long as only phenomenological damping- and friction- models are used. If the implementation is careless, the damping will increase the noise in the system, fluidize the whole assembly or at least distort the results. A further source of noise is the possible degeneration of the unit quaternions for the rotational degrees of freedom: Not only their norm must be constrained, but also the orthogonality to their time-derivative must be enforced by a projection. To our knowledge, this has not been noted in the literature, as in most dynamic simulations, the particles are in perpetual motion. Only when static configurations are investigated, the high noise amplitudes become obvious in the unphysical depletion of the angle of repose. We do not exclude the possibility that such noise will unfavorably affect dynamic results in other fields of computer simulation. Minimizing the noise both for the modeling and the numerics, our three dimensional simulation produced higher angles of repose than purely two dimensional simulations. For low flow rates and high angles of repose, we found consistent density distribution patterns in the experiment and in the simulation for quasi-two dimensional system of particles between walls: a high density column near the middle of the heap reaches to the ground and is surrounded by lower densities regions. In the simulation, we can clearly identify a pressure dip, while for the experiment, we are still hoping that an affordable measurement device becomes available. For the experiment, the density fluctuations were much larger than for the simulation: Future work will have to reveal whether it is due to the fact that the experiment particles are not all strictly convex like the particles in the simulation, or whether it is an defect of the simulation. For high flow rates, where the slope is not straight any more, and the dynamics in the formation is different, the density results are inconclusive but these were also not the slopes for which pressure dips had been reported. All density averages increase towards the ground. Future work will have to show the mechanical principles which cause the arching due to the higher densities. Though improvements will be necessary for both the experiment (better calibration and adjustment) and the simulation (implementation of exact many body friction), qualitatively comparable results have been achieved in a resolution and verisimilitude of the simulation much better than what has been published up to now.

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APPENDIX

A. MODELING OF THE NORMAL FORCE

For a contact pair of particle $\alpha$ and particle $\beta$ (see Fig. 18, left), the contact force $\mathbf{f}_c$ has a normal component $\mathbf{f}_c^n$ and a tangential component $\mathbf{f}_c^t$. The contact force $\mathbf{f}_c^n$ in normal direction consists of the elastic force $\mathbf{f}_e^n$ and a damping force $\mathbf{f}_d^n$. The magnitude of the elastic force $||\mathbf{f}_e^n||$ is obtained from:

$$||\mathbf{f}_e^n|| = YV_0/L_c$$

(13)

in which $||\cdot||$ stands for the norm (or length) of a vector, $Y$ for the Young’s modulus, $V_0$ for the volume of the overlap region, $L_c$ for the characteristic length, which allows to adapt the sound velocity of a space-filling packing to the sound velocity of the continuum for the given Young’s modulus $^{13, 14}$. 

The characteristic length $L_c$ is calculated as:

$$L_c = \frac{4\|r_\alpha\| \cdot \|r_\beta\|}{\|r_\alpha\| + \|r_\beta\|},$$  \hfill (14)

with auxiliary equations, $r_\alpha = c_\alpha - c_\alpha$, $r_\beta = c_\alpha - c_\beta$, where $c_\alpha$, $c_\alpha$, and $c_\beta$ stands for the center of mass of the overlap polyhedron, the particle $\alpha$ and the particle $\beta$ respectively. The magnitude of the damping force $\|f^p_c\|$ is proportional to the change of the volume of the overlap region:

$$\|f^p_c\| = \gamma^r \frac{\sqrt{Y_L} M_{\text{red}}}{L_2 L_c} \delta V_\alpha / \delta t,$$  \hfill (15)

with auxiliary equations, $M_{\text{red}} = \frac{m_\alpha m_\beta}{m_\alpha + m_\beta}$, $L_1 = A_c / L_c$, $L_2 = \sqrt{A_c}$, $A_c = \sum_{i=1}^k A_i$, where $\gamma^r$ is a damping coefficient, $M_{\text{red}}$ the reduced mass and $m_\alpha$ and $m_\beta$ the mass of particle $\alpha$ and $\beta$, $\delta V_\alpha$ the change of the volume of the overlap region over a time interval $\delta t$ and $A_i$ the area of the $i$-th contact triangle (see Fig. 18, right). The normal force $f^p_c$ of the contact is acting at the center of the overlap region $c_\alpha$ and along the direction which is the vector sum of all normals of the contact triangles weighted with the respective area $A_i$,

$$\mathbf{n} = \frac{\sum_{i=1}^s A_i \mathbf{m}_i}{\|\sum_{i=1}^s A_i \mathbf{m}_i\|}$$  \hfill (16)

in which $s$ stands for the number of contact triangles and $\mathbf{m}_i$ for the unit normal vector of the $i$-th contact triangle. Suppose that $\mathbf{n}$ points outside of particle $\alpha$, $\mathbf{n} \cdot r_\alpha < 0$, then the normal contact of particle $\alpha$ is defined as

$$f^p_c = (\|f^p_c\| + \|f^p_\alpha\|) \cdot \mathbf{n},$$  \hfill (17)

while $-f^p_\beta$ for the particle $\beta$. Though $\|f^p_\alpha\|$ is called as magnitude, its value is smaller than zero when $\delta V_\alpha < 0$. A previous study$^{13}$ showed that the following modification is needed:

$$\|f^p_\alpha\| = -\|f^p_\alpha\|, \text{ if } \|f^p_\alpha\| + \|f^p_\alpha\| < 0.$$

B. MODELING OF THE TANGENTIAL FORCE

In two dimensions, the tangential contact force introduced by Cundall and Strack is modeled incrementally$^{11}$: at time $t$, the magnitude of the tangential force $f^t_c$ is given by

$$\|f^t_c(t)\| = \|f^t_c(t - dt)\| + k_t \|v_t\| \cdot dt,$$  \hfill (19)

in which $k_t$ is the tangential stiffness, $v_t$ the tangential velocity; the direction of $f^t_c$ is in the direction opposite to $v_t$; additionally, the magnitude of the tangential force is checked against the maxim possible value $\mu f^p_c$ to apply the rule

$$f^t_c(t) = \text{sgn}(f^t_c(t)) \cdot \mu \|f^p_c(t)\| \text{ if } \|f^t_c(t)\| > \mu f^p_c,$$  \hfill (20)

where sgn is the sign function, $\mu$ the friction coefficient and $f^p_c$ the normal contact force given by Eq. (17). Since the direction of the tangential force is obtained from the tangential velocity, the Cundall-Strack model is a scalar increment of magnitude. However, as shown in Fig. 19, we can
interpret the Cundall-Strack model in a vector projection way: the tangential force from previous time-step \( \mathbf{f}_c^t(t - dt) \) is projected onto the tangential direction of the current time-step along the current contact velocity \( \mathbf{v}_c(t) \) while its magnitude is kept by rescaling the projection of \( \mathbf{f}_c^t(t - dt) \); Then the new tangential force \( \mathbf{f}_c^t \) is obtained by the vector addition of the incremental force \( -k_t \mathbf{v}_t dt \) during the time interval \( dt \) and the magnified projection of previous tangential force \( \mathbf{f}_c^t(t - dt) \).

To generalize the Cundall-Strack model to three dimensions, several issues should be addressed. In three dimensions, the manifold of the tangential movement is two-dimensional \((r_1(t), r_2(t))\), while the actual trajectory of the contact point is three-dimensional \((x(t), y(t), z(t))\). Therefore, we need a way to relate the contact manifold \((r_1(t), r_2(t))\) with the contact trajectory \((x(t), y(t), z(t))\) in a unique way. At the same time, we want to retain the incremental feature of the Cundall-Strack model in two dimensions that the magnitude of the contact force at the previous timestep is used irrespective of a shift in the direction. The three concepts, projection, rescaling, and vector addition, introduced in the vector interpretation are crucial to adapt the Cundall-Strack model for three-dimensional contact problem:

1. Projection: During the advance from time-step \( t - dt \) to time-step \( t \), where we have the new contact normal \( \hat{n}(t) \) and the new tangential velocity \( \mathbf{v}_t(t) \), we project the old tangential force \( \mathbf{f}_c^t(t - dt) \) onto the new tangential plane,

\[
\mathbf{f}_c^t(t - dt) = \mathbf{f}_c^t(t - dt) - (\mathbf{f}_c^t(t - dt) \cdot \hat{n}(t)) \hat{n}(t). \quad (21)
\]

2. Rescaling: We rescale the projection \( \mathbf{f}_c^t(t - dt) \) by the magnitude of the tangential force \( \mathbf{f}_c^t(t - dt) \) at previous time-step \( t - dt \),

\[
\mathbf{f}_c^t(t - dt)^r = \frac{\mathbf{f}_c^t(t - dt) \cdot \mathbf{f}_c^t(t - dt) \cdot \mathbf{f}_c^t(t - dt)}{\mathbf{f}_c^t(t - dt)^p}. \quad (22)
\]

3. Vector addition: the rescaled projection \( \mathbf{f}_c^t(t - dt)^r \) is then added by the incremental vector \( -k_t \mathbf{v}_t dt \) for the time interval \( dt \),

\[
\mathbf{f}_c^t(t) = \mathbf{f}_c^t(t - dt)^r - k_t \mathbf{v}_t dt. \quad (23)
\]

Cut-off is applied, if the results from the vector addition exceeds the maximal friction allowed (the dynamic friction)

\[
\mathbf{f}_c^t(t) = \text{sgn}(\mathbf{f}_c^t(t)) \cdot \mu ||\mathbf{f}_c^t(t)||, \quad \text{if } ||\mathbf{f}_c^t(t)|| > \mu ||\mathbf{f}_c^t(t)||. \quad (24)
\]

Applying the above scheme, we can obtain the three-dimensional vector \( \mathbf{f}_c^t(t) \), which is in the tangential plane of the contact and of incremental property. For the damping force in tangential direction, detailed explanation could be found in the reference [13].

REFERENCES


3) Savage, S. B., “Modeling and Granular Material Boundary Value Problems”, in H. J. Herrmann,


