# Confined granular packings: Structure, stress, and forces 

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#### Abstract

The structure and stresses of static granular packs in cylindrical containers are studied by using large-scale discrete element molecular dynamics simulations in three dimensions. We generate packings by both pouring and sedimentation and examine how the final state depends on the method of construction. The vertical stress becomes depth independent for deep piles and we compare these stress depth profiles to the classical Janssen theory. The majority of the tangential forces for particle-wall contacts are found to be close to the Coulomb failure criterion, in agreement with the theory of Janssen, while particle-particle contacts in the bulk are far from the Coulomb criterion. In addition, we show that a linear hydrostaticlike region at the top of the packings unexplained by the Janssen theory arises because most of the particle-wall tangential forces in this region are far from the Coulomb yield criterion. The distributions of particle-particle and particle-wall contact forces $P(f)$ exhibit exponential-like decay at large forces in agreement with previous studies.


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## I. INTRODUCTION

The formation and structure of granular packs has long been of interest in both the engineering [1] and physics [2] communities. One practical problem has been how to characterize the behavior of granular materials in silos and prevent silo failure. A variety of simulation methods have been developed to describe the stresses on the walls of a silo, though most are confined to two-dimensional (2D) systems. Unfortunately, there is wide disagreement as to the predictive power of these models and the proper approach to take for accurate simulation [3-6]. Those simulations that are carried out in three dimensions usually utilize finite-element methods that provide little information on the internal structure or forces in granular packs [7,8]. Most of the recent 3D discrete-element simulations that have been performed employ periodic boundary conditions in the two directions perpendicular to gravity. Though these studies provide useful information on the internal structure of such packings [9,10], they give no information on vertical stresses or forces at the boundary.

The vertical stress in a silo has traditionally been described by the pioneering 1895 theoretical work of Janssen [11]. This analysis relies on treating a granular pack as a continuous medium where a fraction $\kappa$ of vertical stress is converted to horizontal stress. The form of the vertical stress appears if one assumes that the frictional forces between particles and walls are at the Coulomb failure criterion: $F_{t}$ $=\mu_{w} F_{n}$, where $F_{t}$ is the tangential friction force, $F_{n}$ is the normal force at the wall, and $\mu_{w}$ is the coefficient of friction for particle-wall contacts. Numerous improvements have

[^0]been added over time, but in many cases their effect on the theory is small [1]. Recently, experiments have been carried out on granular packs in silos to test the suitability of Janssen's theory in ideal conditions. These studies [12,13] measured the apparent mass at the bottom of the silo as a function of the filling mass. They found the best agreement with a phenomenological theory containing elements of Janssen's original model, which we describe in more detail in Sec. IV.

We present here large-scale 3D discrete particle, molecular dynamics simulations of granular packings in cylindrical containers (silos). Our aim is to understand the internal structure and vertical stress profiles of these granular packings and reconcile our results with existing theory. A variety of methods simulating pouring and sedimentation are used to generate the packings. We show how the different methods of filling the container affect the final bulk structure of the packings. We evaluate the suitability of the Janssen theory to the observed vertical stress profiles and test the validity of its assumptions. We show that the majority of particle-wall contact forces are close to the Coulomb failure criteria, whereas particle-particle forces in the bulk are far from yield. Finally, we show that the distribution of contact forces in these packings show exponential-like tails, in the bulk, at the side walls and at the base $[14,15]$.

The simulation method is presented in Sec. I, where we also discuss the various methods that were used to generate the packings. In Sec. II, we show how the different methods affect the bulk structure of the packings. Sec. III presents the vertical stress profiles and discusses their characteristics and we compare our results to the classical theory of Janssen as well as two modified forms of the Janssen analysis. In Sec. IV we present our results on the distribution of forces and test the Janssen prediction of Coulomb failure at the walls of the cylinder. We conclude and summarize the work in Sec. V.

## II. SIMULATION METHOD

We present molecular dynamics (MD) simulations in three dimensions on model systems of $N$ monodispersed spheres of diameter $d$ and mass $m$. We vary $N$ from 20000 to 200000 particles. The system is constrained by a cylinder of radius $R$, centered on $x=y=0$, with its axis along the vertical $z$ direction. The cylinder is bounded below with a flat base at $z=0$. In some cases, a layer of randomly arranged immobilized particles approximately $2 d$ high rests on top of the flat base to provide a rough base. The cylinders used vary in size from $R=10 d$ to $20 d$. This work builds on previous MD simulations of packings with periodic boundary conditions in the $x y$ plane [10].

The spheres interact only on contact through a springdashpot interaction in the normal and tangential directions to their lines of centers. Contacting spheres $i$ and $j$ positioned at $\mathbf{r}_{i}$ and $\mathbf{r}_{j}$ experience a relative normal compression $\delta=\mid \mathbf{r}_{i j}$ $-d \mid$, where $\mathbf{r}_{i j}=\mathbf{r}_{i}-\mathbf{r}_{j}$, which results in a force

$$
\begin{equation*}
\mathbf{F}_{i j}=\mathbf{F}_{n}+\mathbf{F}_{t} . \tag{1}
\end{equation*}
$$

The normal and tangential contact forces are given by

$$
\begin{align*}
& \mathbf{F}_{n}=f(\delta / d)\left(k_{n} \delta \mathbf{n}_{i j}-\frac{m}{2} \gamma_{n} \mathbf{v}_{n}\right),  \tag{2}\\
& \mathbf{F}_{t}=f(\delta / d)\left(-k_{t} \boldsymbol{\Delta} \mathbf{s}_{t}-\frac{m}{2} \gamma_{t} \mathbf{v}_{t}\right), \tag{3}
\end{align*}
$$

where $\mathbf{n}_{i j}=\mathbf{r}_{i j} / r_{i j}$, with $r_{i j}=\left|\mathbf{r}_{i j}\right| . \mathbf{v}_{n}$ and $\mathbf{v}_{t}$ are, respectively, the normal and tangential components of the relative surface velocity, and $k_{n, t}$ and $\gamma_{n, t}$ are elastic and viscoelastic constants, respectively. $f(x)=1$ for Hookean (linear) contacts, while for Hertzian contacts $f(x)=\sqrt{x} . \Delta \mathbf{s}_{t}$ is the elastic tangential displacement between spheres, obtained by integrating tangential relative velocities during elastic deformation for the lifetime of the contact. The magnitude of $\Delta \mathbf{s}_{t}$ is truncated as necessary to satisfy a local Coulomb yield criterion $F_{t} \leqslant \mu F_{n}$, where $F_{t} \equiv\left|\mathbf{F}_{t}\right|$ and $F_{n} \equiv\left|\mathbf{F}_{n}\right|$ and $\mu$ is the particle-particle friction coefficient. Frictionless spheres correspond to $\mu=0$. Particle-wall interactions are treated identically, but the particle-wall friction coefficient $\mu_{w}$ is set independently. A more detailed description of the model is available elsewhere [16].

Most of these simulations are run with a fixed set of parameters: $k_{n}=2 \times 10^{5} \mathrm{mg} / \mathrm{d}, k_{t}=\frac{2}{7} k_{n}$, and $\gamma_{n}=50 \sqrt{g / d}$. For Hookean springs we set $\gamma_{t}=0$. For Hertzian springs, $\gamma_{t}$ $=\gamma_{n}$ [17]. In these simulations, it takes far longer to drain the energy out of granular packs, using the Hertzian force law, since the coefficient of restitution $\epsilon$ is velocity dependent [18] and goes to zero as the velocity goes to zero. We thus focused on Hookean contacts, which for the above parameters give $\epsilon=0.88$. The convenient time unit is $\tau$ $=\sqrt{d / g}$, the time it takes a particle to fall its radius from rest under gravity. For this set of parameters, the time step $\delta t$ $=10^{-4} \tau$. The particle-particle friction and particle-wall friction are the same: $\mu=\mu_{w}=0.5$, unless stated otherwise.


FIG. 1. Formation of a packing of $N=20000$ spheres in a cylindrical container of radius $10 d$ onto a flat base. The packing is constructed by pouring, using method P 1 , from a height of 70 d . The configurations shown are for early, intermediate, and late times. The final static pile has $\phi_{f}=0.62$.

All of our results will be given in dimensionless units based on $m, d$, and $g$. Physical experiments often use glass spheres of $d=100 \mu \mathrm{~m}$ with $\rho=2 \times 10^{3} \mathrm{~kg} / \mathrm{m}^{3}$. In this case, the physical elastic constant would be $k_{\text {glass }} \sim 10^{10} \mathrm{mg} / \mathrm{d}$. A spring constant this high would be prohibitively computationally expensive, because the time step must have the form $\delta t \propto k^{-1 / 2}$ for collisions to be modeled effectively. We have found that running simulations with larger $k$ 's does not appreciatively change the physical results [16].

We use a variety of techniques to generate our static packings. In method P1, we mimic the pouring of particles at a fixed height $Z$ into the container. For computational efficiency, a group of $M$ particles is added to the simulation on a single time step as if they had been added one by one at random times. This is done by inserting the $M$ particles at nonoverlapping positions within a thin cylindrical region of radius $R-d$ that extends in $z$ from $Z$ to $Z-d$. The $x, y$, and $z$ coordinates of the particles are chosen randomly within this insertion region. The height of insertion $z$ determines the initial $z$ velocity $v_{z}$ of the particle- $v_{z}$ is set to the value it would have after falling from a height $Z$. After a time $\sqrt{2} \tau$, another group of $M$ particles is inserted. This methodology generates a steady stream of particles, as if they were poured continuously from a hopper (see Fig. 1). The rate of pouring is controlled by setting $M$ to correspond to a desired volume fraction of particles within the insertion region. For example, for an initial volume fraction of $\phi_{i}=0.13$ and $R=10 d$, the pouring rate is $\approx 45$ particles per $\tau$.

Method P 2 is similar, but the insertion region moves in $z$ with time, so that the particles are inserted at roughly the same distance from the top of the pile over the course of the simulation. The insertion region is the same as in method P1,
with thickness $\delta z=1$ and radius $R-d$. For the results presented here, the initial height is $10 d$ and the insertion point moves upward with velocity $v_{\text {ins }}=0.15 d / \tau \hat{z}$. For 50000 particles, the pouring region rises $150 d$ over the course of the simulation. A 50000 particle pack in a $R=10 d$ cylinder is roughly $140 d$ high, making this a reasonable rate for pouring in particles at approximately the same height over a long run. Different configurations were produced by using different random number seeds to place the particles in the insertion region. These two methods are similar to the homogeneous "raining" methods used in experiments [20].

We also prepare packings that simulate particle sedimentation. In this method nonoverlapping particles with a packing fraction $\phi \approx 0.13$ are randomly placed in a cylindrical region of radius $R-d$ extending from $z=10 d$ to the top of the simulation box. This tall, dilute column of particles is then allowed to settle under the influence of gravity in the presence of a viscous damping term-each particle $i$ feels an additional Stokes drag force $F_{i}^{d a m p}=-b v_{i}$, with the damping coefficient $b=0.20 m \sqrt{g / d}$. The terminal velocity $v_{\text {term }}$ $=m g / b=5 \sqrt{d g}$ is the same velocity as that of a free-falling particle that has fallen $25 d / 2$ from rest. This method, which we refer to as S2, closely approximates sedimentation in the presence of a background fluid. It also shares some similarities with method P2, being very similar to pouring particles from a constant height above the pile. We also run the simulation with no viscous damping, $b=0$, and refer to this as method S1. In both cases, we start from the same initial configuration of particles but give the particles different random initial velocities ranging from $-10 d / \tau$ to $10 d / \tau$ for the horizontal components and $-10 d / \tau$ to 0 for the vertical component to create different configurations.

In all cases, the simulations were run until the kinetic energy per particle was less than $10^{-8} \mathrm{mgd}$. The resultant packing is considered quiescent and used for further analysis [10]. For method S1, the free-fall portion of the simulation is a small fraction of the simulation time, with the largest fraction of the simulation time devoted to dissipation of the local vibrations of particles in contact. For the other three methods, the packs form as the pouring continues and lose their kinetic energy very soon after the last particle settles on top of the pack.

These simulations were performed on a parallel cluster computer built with DEC Alpha processors and Myrinet interconnects, using a parallel molecular dynamics code optimized for short-range interactions $[16,19]$. A typical simulation to create a 50000 particle $R=10 d$ packing through pouring takes $5 \times 10^{6}$ time steps to complete and requires roughly 40 CPU hours on 50 processors.

Figure 1 shows a sample progression of our simulations for method P1, while Fig. 2 shows similar results for method S2, which are the two methods we focus on in this paper. Both the cases show a series of three snapshots over the course of the formation of the pack $[21,22]$.

## III. STRUCTURE OF THE PACKINGS

The packings generated by these four methods had similar bulk characteristics, though there were some differences in


FIG. 2. Lower portion of the packing of $N=20000$ spheres in a cylindrical container of radius $R=10 \mathrm{~d}$. The packing is supported by a rough fixed bed (darker particles) and is constructed by sedimentation, using method S2. The three configurations shown are the initial configurations with volume fraction $\phi_{i}=0.13$, an intermediate one, and the final static pile with $\phi_{f} \approx 0.60$.
the final packing fraction $\phi_{f}$ and coordination number $n_{c}$. In all cases, the bulk properties of the packings were the same for different random initial conditions using the same method. For a given set of initial conditions such as pouring rate, pouring height, or initial density, the height of the resultant packing was the same to within $d / 4$. The resulting packing fraction $\phi$ and coordination number $n_{c}$ within the pack were reproducible for a given set of initial conditions. Because of this, we frequently averaged over multiple runs with different random initial conditions to improve statistics in the presentation that follows.

Small differences in the physical structure of the packs were observed that depend slightly on the generation method. In general, packings created by pouring were denser than those created by sedimentation. For otherwise identical 50000 particle packings in a cylinder of radius $R=10 d$ with default parameters, packings created using methods $P 1$ had an average volume fraction $\phi_{f} \approx 0.621$ and for P 2 had an average volume fraction of $\phi_{f} \approx 0.614$, using a pouring rate of 45 particles per $\tau$. Those created using method S1 had an average volume fraction of $\phi_{f} \approx 0.597$ and those using method S2 had an average volume fraction of $\phi_{f} \approx 0.594$. These differences were reproducible over different initial conditions. The difference between pouring and sedimentation seems to arise from the much longer times involved in pouring, because the energies involved in both methods are not dissimilar. The longer time scales required to form packs through pouring seem to allow particles more time to settle and rearrange, thus creating denser packs. Sedimentation occurs over much faster time scales and seems to lock the particles into metastable configurations that are less dense. For method P1, increasing the height from which the particles were poured also increased the density of the final


FIG. 3. Final average packing fraction $\phi_{f}$ as a function of pouring rate $v_{p}$ (in units of $1 / \tau$ ). Results are for packings of 50000 particles with $R=10 d$ poured from a height of $180 d$ with method P1. The line is a guide to the eye. Slower pour rates create denser packings.
pack, though the effect was slight. This effect probably arises from the greater kinetic energy of the particles when they hit the pack, which allows them to explore more phase space, resulting in denser packs. The pouring rate also affects the final density $\phi_{f}$, with faster pouring rates producing looser packings, as shown in Fig. 3. This is the same effect as above, with faster pouring rates forcing particles into looser metastable configurations. The final packing fraction $\phi_{f}$ 's for method P2 are consistently lower than those for method P1. This is due to the change in kinetic energy, because the kinetic energy of pouring particles in method P2 is much smaller than in P1. As was reported earlier for periodic systems [10], more dilute initial packing fractions $\phi_{i}$ result in larger final packing fractions $\phi_{f}$, and we see this behavior also for our simulations using method S 1 . This is the same effect as increasing the pouring height, because more dilute columns with smaller $\phi_{i}$ are also taller and thus have greater potential energy. In model S2 the final velocity of the falling particles is limited by the drag to a small terminal velocity. This removes any excess kinetic energy and the final packing fractions of these packings are independent of the initial state. Finally, the force law chosen also has a very slight effect on the final structure of the pack. Replacing the Hookean force law with Hertzian results in a slightly denser pack. We thus affirm the history dependence of granular packings: the structure of the resultant packing is dependent on the particular method used to generate it [20].

We find that significant particle ordering is seen at the cylinder walls, but this boundary effect penetrates only a few diameters into the bulk for cylinders of various radii. Figure 4 shows the final packing fraction as a function of radius for a set of packings created, using the same parameters in cylinders of different radii using method S2. In all these cases $\phi_{f}$ quickly approaches the bulk value irrespective of the size of the container. In addition, the decay length $\nu$ is independent of size and extends over $\nu \approx 4 d$ for all $R$.

Previous studies of granular packings have been concerned with the stability of packings [9,23-25]. The stability of a packing is based on the average number of contacts per


FIG. 4. Final volume fraction $\phi_{f}$ of packings as a function of radius for packings of $N=50000$ and $R=10, N=82000$ and $R$ $=15$, and $N=144000$ and $R=20$, using method S2. The effects of the wall penetrate about $4 d$ in each case.
particle-the coordination number $n_{c}$. The theoretical limit for stability of particles with friction is $n_{c}=4$ (Ref. [26]). Packings with $n_{c}=4$ are said to be isostatic, while those with $n_{c}>4$ are hyperstatic-they have more contacts than are needed for mechanical stability. A previous study [25] of packings with horizontal periodic boundary conditions using the same model concluded that frictional packings are always hyperstatic. Using methods S1 and S2, we see identical results for $\phi_{f}$ and $n_{c}$ to those previous measurements in the inner core of our packings for particles more than $5 d$ from the outer wall, which should remove any ordering effects originating from the wall. Packings generated by methods P1 and P2 are also hyperstatic. This suggests that the previous conclusions of hyperstaticity also apply in the bulk of silos and that the walls have only a small effect on the physical structure of packings. The method used to create the packings seems to have a much larger effect.

## IV. DISTRIBUTION OF STRESSES

Of particular interest in the construction of silos is the distribution of stresses in a cylindrical packing [1]. In a liquid, hydrostatic pressure increases with depth. Granular materials support shear, so the side walls of a container can support some of this pressure. The problem of the resultant vertical stress in a silo after filling has a long history, beginning with Janssen in 1895. Janssen's analysis [11,27] of the stress in a silo rested on three assumptions: the granular particles are treated as a continuous medium, a vertical stress $\sigma_{z z}$ applied to the material automatically generates a horizontal stress $\sigma_{h}=\kappa \sigma_{z z}$, and the frictional forces between the particles and the wall are at the point of Coulomb failure ( $F_{t}=\mu_{w} F_{n}$ ), where the frictional force can no longer resist tangential motion of the particle and has a specific direction. In our case, this direction is upward as the particles settle. Using our simulations we can test some of these assumptions.

For a cylindrical container of radius $R$ with static wall friction $\mu_{w}$ and granular pack of total height $z_{0}$, the Janssen analysis predicts the vertical stress $\sigma_{z z}(z)$ at a height $z$ is


FIG. 5. Vertical stress $\sigma_{z z}$ in units of $\mathrm{mg} / \mathrm{d}^{2}$ for $N=20000$ to 60000 packings with a rough base, using $\mu=\mu_{w}=0.5$ and $R$ $=10 \mathrm{~d}$ for method S2. Data for each value of $N$ is averaged over six runs.

$$
\begin{equation*}
\sigma_{z z}(z)=\rho g \bar{l}\left[1-\exp \left(-\frac{z_{0}-z}{l}\right)\right], \tag{4}
\end{equation*}
$$

where the decay length $l=R / 2 \kappa \mu_{w} . \kappa$ represents the fraction of the weight carried by the side walls, $\rho$ is the volumetric density, and $z_{0}$ is the top of the packing. In our case, $\rho=\phi_{f} \rho_{p}$, where $\rho_{p}=6 \mathrm{~m} / \pi d^{3}$ is the density of a single particle. Standard Janssen analysis mandates that $l=\bar{l}$, so that $l$ is the only free parameter. As seen below in Fig. 6, this single parameter formula does not provide a good qualitative fit to our data. We have generalized the formula to include a two-parameter fit with $l \neq \bar{l}$. This separates the asymptote from the decay length. This generalization is similar to that proposed by Walker to address the experimental fact that stresses are not uniform across horizontal slices, as was assumed in the original Janssen analysis [28,29].

Another two-parameter fit was proposed by Vanel and Clément [12] to reconcile their experimental findings with the Janssen theory. The fit assumes a region of perfect hydrostaticity, followed by a region that conforms to the Janssen theory:

$$
z_{0}-z<a: \sigma_{z z}(z)=\rho g\left(z_{0}-z\right)
$$



$$
\begin{equation*}
z_{0}-z>a: \sigma_{z z}(z)=\rho g\left\{a+l\left[1-\exp \left(-\frac{z_{0}-z-a}{l}\right)\right]\right\} \tag{5}
\end{equation*}
$$

This hydrostatic region is also predicted by a model of Evesque and de Gennes [30].

Vertical stress profiles of packings for different numbers of particles using method S2 are shown in Fig. 5. As the height of the packing increases, the region of heightindependent stress also increases. We estimate that a ratio of height to radius of $h / R \approx 6$ is required to see this behavior, though this may be somewhat dependent on our cylindrical geometry and also the dimensionality of the system, since this ratio is smaller than that observed in 2D [3,35]. There is a slight increase in the vertical stress at the base of all of these packings. This is a generic feature of our packings, visible in packings with rough and flat bases, and is a boundary effect at the base. We ignore this small region in our subsequent analyses. We show a fit of the $N=50000$ stress profile to the Janssen formula (4) in Fig. 6(a). We obtain the fit by setting the asymptote $\rho g \bar{l}$ equal to the value of the stress in the height-independent region. This section is independent of depth and thus is the controlling factor for the Janssen fit. We used the standard $\chi^{2}$ measure of goodness of fit to evaluate the fit, where

$$
\chi^{2}=\sum_{i=1}^{N} \frac{\left(y_{i}-x_{i}\right)^{2}}{N-1}
$$

$N$ is the number of data points, $x_{i}$ is the simulation data, and $y_{i}$ are the points from the fit. In this and subsequent fits, we do not use the bottom $25 d$ of the cylinder, as the uptick of the stress there is a boundary effect. All fit parameters are summarized in Table I. The Janssen fit is relatively poor ( $\chi^{2}=10.5$ ), and it substantially underpredicts the stress in the turnover region. As in the experimental data by Vanel and Clément [12], the hydrostatic region is larger than predicted by the standard Janssen analysis. We also fit our stress profile to the modified Janssen form $(l \neq \bar{l})$, taking $\bar{l}$ from the asymptote as before and fitting $l$ as a free parameter. This fit is better $\left(\chi^{2}=1.03\right)$. However, this form also underpredicts the size of the linear region and overshoots the data for large $z$, as shown in Fig. 6(b). As the stress increases linearly with $z$


FIG. 6. Vertical stress $\sigma_{z z}$ in units of $m g / d^{2}$ for $N=50000$, using method S 2 . The data are represented by the diamonds. The dotted line is a fit to the Janssen expression with $l=\bar{l}$, Eq. (4). The dashed line is a fit to the modified Janssen expression with $l \neq \bar{l}$. The solid line is a fit to the two parameter theory, Eq. (5). (b) is a blowup of the turnover region on the right side of (a).

TABLE I. Results of the fits for vertical stress in packings, using method S2 and the corresponding physical parameters.

| Packing friction | Janssen | Modified Janssen | Vanel-Clément |
| :--- | :---: | :---: | :---: |
| $\mu=0.5$ | $\chi^{2}=10.5$ | $\chi^{2}=1.03$ | $\chi^{2}=0.092$ |
| $\mu_{w}=0.5$ | $\kappa=0.404$ | $\kappa=0.677$ | $\kappa=1.14$ |
|  | $l / d=24.8$ | $l / d=14.8$ | $/ / d=8.76$ |
|  |  | $\bar{l} / d=24.8$ | $a / d=16.0$ |
| $\mu=0.5$ | $\kappa=0.168$ | $\kappa=0.218$ |  |
| $\mu_{w}=2.0$ |  | $l / d=14.9$ | $l / d=11.5$ |
|  |  |  |  |
|  |  | $l / d=22.7$ | $a / d=11.5$ |

near the top of the packing, it is not surprising that the best fit was obtained with the two-parameter Vanel-Clément form, Eq. (5), with a $\chi^{2}=0.092$. These results are qualitatively in agreement with the results obtained by Vanel and Clément: we obtain $\kappa$ 's greater than 1 for the two-parameter fit and $\kappa$ 's smaller than one for the standard Janssen fit. It is difficult to provide a direct prediction for the value of $\kappa$ we expect [1]. The latter two fits (modified Janssen and the two-region fit) do not have a theoretical basis, but clearly represent the data much better. There is a substantial region of linear hydrostatic pressure at the top of the packing that both the classical and modified Janssen theory do not account for.

We find similar results for all other methods except S1. Method S1 is somewhat unphysical, since the particles hit the packing with increasing kinetic energy as the simulation progresses. The vertical stress we observe in this case is substantially larger than that observed for other methods and is noticeably peaked near the top of the sample. This arises because the large velocities of accelerating particles excessively compact the pack at impact. The pack then attempts to relax, but the side walls exert their own pressure on the pack, keeping it in its "stressed" position, yielding a total pressure greater than hydrostatic and freezing in this kinetic stress. Although there is a large difference in the stress profiles between packings generated by method S1 and S2, $\phi_{f}$ of the former is only slightly larger.

To test the underlying assumptions of the Janssen analysis, we varied the particle-wall friction $\mu_{w}$. First, we set $\mu_{w}=0$, which removed any particle-wall friction. This prevents the side walls from supporting any weight and is similar to unconfined packings. The result is a vertical stress that increases linearly with height, exactly as in the hydrostatic case and as expected from the Janssen analysis. Another test was to increase the particle-wall friction, setting $\mu_{w}=2.0$. This ensures a very high limit for the Coulomb failure criterion. We compare the stress profile of the $\mu_{w}=2.0$ case to our standard $\mu_{w}=0.5$ case in Fig. 7, both with $\mu=0.5$. The higher wall-friction case has a lower height-independent stress, because the larger the $\mu_{w}$, the more the walls can support. However, this difference is not large, and using $\mu_{w}=2.0$ to obtain $\kappa$ values results in unreasonably low values, as seen in Table I. The modified Janssen form gives $\kappa$ $=0.168$, and the two-parameter fit gives $\kappa=0.218$. $\kappa$ should be a feature of the material used and not vary greatly when the wall friction is changed [1]. All of these fits use part of


FIG. 7. Vertical stress $\sigma_{z z}$ in the top part of $N=50000$ packings, with $\mu_{w}=2$ (diamonds) and $\mu_{w}=0.5$ (open circles), both using method S2. The dotted line is a fit to the $\mu_{w}=2$ data with the modified Janssen formula with $l \neq \bar{l}$ and the straight line is a fit to the same with the two-parameter Vanel-Clément formula.
the Janssen theory, and the discrepancy in $\kappa$ arises because the third assumption of the Janssen analysis is not satisfied: the tangential forces at the wall for the $\mu_{w}=2.0$ case are considerably less than $\mu_{w} F_{n}$ and thus far from the Coulomb failure criterion, as seen in Sec. V.

We also analyzed stress profiles in larger cylinders of radius $R=15 d$ and $R=20 d$. A comparison of different stress profiles is shown in Fig. 8(a) for method S2 and in Fig. 8(b) for method P1. The wider cylinders have larger stresses in their asymptotic region because the amount of material they must support is larger. These profiles show that the crossover to height-independent pressure occurs approximately at height $\approx 6 R$, irrespective of pouring method. In all cases, note the linear, hydrostaticlike stress region at the top of the pile.

Methods P1 and P2 had similar stress profiles. Pouring the particles from different heights had a small effect on the stress profiles. Increasing the height from which the particles were poured increased the internal stress. This arises from their higher potential energy. The increase in stress is much greater than the small difference in packing fraction observed between these packings. We also varied the pouring rate for these packings and found this had little or no effect on the stress profiles. This leads us to conclude that internal stress in a packing is primarily affected by the particle-wall friction coefficient $\mu_{w}$, the geometry of the cylinder, and the amount of potential energy that the particles possess, here represented by height of pouring. Changes in other parameters that can affect characteristics of the pack such as packing fraction but do not change the potential energy have little effect on the stress profiles.

## V. DISTRIBUTION OF FORCES

Numerous experiments have been done to measure the distribution of normal contact forces $P\left(f_{n}\right)$ in granular packings, where $f_{n}=F_{n} / \bar{F}_{n}$ and $\bar{F}_{n}$ is the average normal force. These packings all show approximately exponential tails in $P\left(f_{n}\right)$ for large forces $f_{n}>1$ [14,31]. Unfortunately, in the


FIG. 8. Comparison of the resultant stress for packings created with cylinders of different radii $R$. (a) For sedimentation method S2, the highest stress is for an $R=20 d$ cylindrical packing with $N=144000$ particles, the second highest is for an $R=15 d$ cylindrical packing with 82000 particles, and the lowest is for 50000 particles and $R=10 d$. (b) For pouring method P 1 , the highest stress is for an $R=20 d$ packing with $N=200000$ particles, next highest is for an $R=15 d$ packing with 120000 particles, and the lowest is for an $R=10 d$ packing with 50000 particles. All the results are a single run except the two 50000 -particle systems, which are averaged over six runs.
experiments it is difficult to probe the distribution of forces in the interior of the pack. We measure $P\left(f_{n}\right)$ in both the bulk of packings and along the side walls and flat bottoms of the cylinder, shown in Fig. 9. These packings were created using method P1 with $\mu_{w}=0.5$, though the form of the tail of $P(f)$ is remarkably robust to changes in method or parameters. In addition, we see the same form of the distribution for the tangential $P\left(f_{t}\right)$, as reported in simulations with periodic packings [32]. These $P\left(f_{n}\right)$ curves are quite consistent with previous measurements of $P\left(f_{n}\right)$ [14] at the base of a packing. In addition, these results indicate the form of $P(f)$ inside a packing is not qualitatively different from that taken on the edge or bottom of a cylinder. Recent experiments on emulsions have found similar distributions for $P(f)$ in the bulk $[33,34]$. This implies that the measurements of $P(f)$ taken by an experiment using forces at the edge give a good picture of the distribution in the packing as a whole.

Using our force measurements, we can further test the reliability of the Janssen assumptions by checking whether the tangential forces at the wall are actually at the Coulomb yield criterion $F_{t}=\mu_{w} F_{n}$. We define $\zeta=F_{t} / \mu F_{n}$ in the bulk of the packing and $\zeta=F_{t} / \mu_{w} F_{n}$ for forces at the wall. If a specific force is at the Coulomb failure criterion, $\zeta=1$. By examining the distribution of forces in the interior of our
packings, we find that almost no particle-particle contacts are at the Coulomb criterion irrespective of method or parameters, as shown in Fig. 10(a). When we examine the particlewall forces in the height-independent stress region, the forces are much closer to the Coulomb criterion. For $\mu=\mu_{w}$ $=0.5$, the majority of the tangential forces are close to the Coulomb criterion for different methods. When $\mu>\mu_{w}$, we find that most of the particle-wall tangential forces are also near the Coulomb failure criterion. However, for extremely high-friction walls $\left(\mu=0.5, \quad \mu_{w}=2.0\right)$, most tangential forces are not at the Coulomb criterion, as shown in Fig. 10(b). The peak in the particle-wall distribution occurs near $F_{t}=\mu F_{n}$. This suggests that there is an effective $\mu_{w, e f f}$, which is the lesser of the original $\mu_{w}$ and $\mu$. If we redo the modified Janssen fit as before for the $\mu_{w}=2.0$ case and use an effective $\mu_{w, e f f}=0.5$, as determined from our contact forces, we obtain $\kappa=0.72$, a value close to our previous value for $\mu_{w}=0.5$, which is what one would expect. It appears that the wall does not support in meaningful numbers larger tangential forces than those between particles, because particles slip and move against other particles and thus detach from the wall regardless of the high $\mu_{w}$. This suggests that when the particle-particle friction $\mu$ and particle-wall friction $\mu_{w}$ are matched, the majority of the particle-wall


FIG. 9. Distribution of normal $f_{n}$ and tangential $f_{t}$ contact forces for a packing of 50000 particles generated, using method P1. Bulk forces are represented as open circles, forces between particles and side wall are represented as filled-in triangles, and forces between particles and the flat base are represented as filled-in squares. All forces exhibit the same quasiexponential tails.


FIG. 10. Probability distributions $P(\zeta)$ in the height-independent pressure region in the bulk of the packing (a) and at the side walls (b), each normalized by its maximum value $P\left(\zeta_{\max }\right) . \zeta=F_{t} / \mu F_{n}$ in (a) and $F_{t} / \mu_{w} F_{n}$ in (b). Forces in the bulk are far from the Coulomb failure criterion, while many of those at the walls are very close to it. The legends for (a) and (b) are the same.
forces at the wall are close to the Coulomb failure criterion. One exception occurs for large $\mu, \mu=\mu_{w}=1.0$. This allows very large frictional forces, and it seems likely (as observed in other simulations [10]) that even though the wall and particles can support larger tangential forces in principle, no tangential forces of this magnitude are generated. This information about the Coulomb failure criterion in the depthindependent pressure region gives us no information on the extended hydrostaticlike region at the top of the pile.

We have also analyzed the linear hydrostatic region specifically and show our results in Fig. 11, using $\zeta$ $=F_{t} / \mu_{w} F_{n}$ as in the earlier figures. In this region, few of the forces at the wall are near the Coulomb criteria, regardless of the value of $\mu$ and $\mu_{w}$. This is a partial explanation for why the Janssen analysis does not apply in this region. The walls in this region support very little weight and thus the stress profile in this region is similar to the linear hydrostatic case. The nature of the transition between this hydrostaticlike region and the bulk region remains to be explored.

## VI. CONCLUSIONS

We have used large-scale simulations to study granular packings in cylindrical containers. We used a variety of


FIG. 11. Probability distributions $P(\zeta)$ at the side wall in the linear hydrostatic region at the top of the packing with $\mu=\mu_{w}$ $=0.5$, each normalized by its maximum value $P\left(\zeta_{\max }\right) ; \zeta$ $=F_{t} / \mu_{w} F_{n}$. The solid line is the data for method S 2 and the dashed line the data for method P1. In contrast to the behavior in the height-independent pressure region, the forces at the walls are far from the Coulomb failure criterion in all cases.
methods to generate these packings and studied the effects of packing preparation on the final static packing. We show that the classical Janssen analysis does not fully describe our packings, but that slight modifications to the theory of Janssen enable us to describe our packings well. In addition, we explore some of the assumptions of Janssen and show that when the particle-particle and particle-wall friction interactions are balanced, the particle-wall interaction close to the wall is at the Coulomb failure criterion. We show that the anomalous hydrostatic region at the top of our packings arises because the forces at the wall are far from the Coulomb failure criterion and thus support very little weight, in contrast to the results deeper in the packing. We also demonstrate that the distribution of forces in our packings is consistent with previous results in both experiment and simulation not only in the bulk but also at the walls and base.

Much of the literature on vertical stress profiles in silos focuses on 2D systems. The stress profiles of packings are strongly influenced by the dimensionality of the system and we explore the crossover between 2D packings, quasi-2D packings of particles in flat cells, and fully 3D packings in another work [35].

While this work was being prepared, we became aware of two new granular experiments that find a Janssen form for the vertical stress [36,37]. These experiments use either a movable base or movable cylindrical walls to mobilize the grains more fully, producing a more Janssen-like vertical stress. The present simulations are much closer to the VanelClément experiments [12,13], which were taken after the packing had settled into its final state.

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[1] R. M. Nedderman, Statics and Kinematics of Granular Materials (Cambridge University Press, Cambridge, 1992).
[2] H.M. Jaeger, S.R. Nagel, and R.P. Behringer, Rev. Mod. Phys. 68, 1259 (1996).
[3] S. Masson and J. Martinez, Powder Technol. 109, 164 (2000).
[4] J.M.F.G. Holst, J.Y. Ooi, J.M. Rotter, and G.H. Rong, J. Eng. Mech. 125, 94 (1999).
[5] J.M.F.G. Holst, J.Y. Ooi, J.M. Rotter, and G.H. Rong, J. Eng. Mech. 125, 104 (1999).
[6] A.M. Sanad, J.Y. Ooi, J.M.F.G. Holst, and J.M. Rotter, J. Eng. Mech. 127, 1033 (2001).
[7] J.F. Chen, S.K. Yu, J.Y. Ooi, and J.M. Rotter, J. Eng. Mech. 127, 1058 (2001).
[8] D. Guines, E. Ragneau, and B. Kerour, J. Eng. Mech. 127, 1051 (2001).
[9] H.A. Makse, D.L. Johnson, and L.M. Schwartz, Phys. Rev. Lett. 84, 4160 (2000).
[10] L.E. Silbert, D. Ertaş, G.S. Grest, T.C. Halsey, and D. Levine, Phys. Rev. E 65, 031304 (2002).
[11] H.A. Janssen, Z. Ver. Dt. Ing 39, 1045 (1895).
[12] L. Vanel and E. Clément, Eur. Phys. J. B 11, 525 (1999).
[13] L. Vanel, P. Claudin, J.-P. Bouchaud, M. Cates, E. Clément, and J.P. Wittmer, Phys. Rev. Lett. 84, 1439 (2000).
[14] D.L. Blair, N.W. Mueggenburg, A.H. Marshall, H.M. Jaeger, and S.R. Nagel, Phys. Rev. E 63, 041304 (2001).
[15] D.M. Mueth, H.M. Jaeger, and S.R. Nagel, Phys. Rev. E 57, 3164 (1998).
[16] L.E. Silbert, D. Ertaş, G.S. Grest, T.C. Halsey, D. Levine, and S.J. Plimpton, Phys. Rev. E 64, 051302 (2001).
[17] In the Hookean case, energy drains out of the pile efficiently and additional damping is not required. For Hertzian contacts, tangential damping is required to allow the energy in the pile to dissipate in a reasonable computational time.
[18] J. Schäfer, S. Dippel, and D.E. Wolf, J. Phys. I 6, 5 (1996).
[19] S.J. Plimpton, J. Comput. Phys. 117, 1 (1995).
[20] L. Vanel, D. Howell, D. Clark, R.P. Behringer, and E. Clément, Phys. Rev. E 60, R5040 (1999).
[21] E.A. Merritt and D.A. Bacon, Methods Enzymol. 277, 505 (1997).
[22] These figures were created using the raster3d program version 2.6e.
[23] T.G. Mason, M.-D. Lacasse, G.S. Grest, D. Levine, J. Bibette, and D.A. Weitz, Phys. Rev. E 56, 3150 (1997).
[24] C.S. O'Hern, S.A. Langer, A.J. Liu, and S.R. Nagel, Phys. Rev. Lett. 88, 075507 (2002).
[25] L.E. Silbert, D. Ertaş, G.S. Grest, T.C. Halsey, and D. Levine, Phys. Rev. E 65, 051307 (2002).
[26] S. Alexander, Phys. Rep. 296, 65 (1998).
[27] L. Rayleigh, Philos. Mag. 11, 129 (1906).
[28] D.M. Walker, Chem. Eng. Sci. 21, 975 (1966).
[29] K.J. Walters and R.M. Nedderman, Chem. Eng. Sci. 28, 779 (1973).
[30] P. Evesque and P.-G. de Gennes, C. R. Acad. Sci. Paris 326, 761 (1998).
[31] J.H. Snoeijer, M. van Hecke, E. Somfai, and W. van Saarloos, e-print cond-mat/0204277.
[32] L.E. Silbert, G.S. Grest, and J.W. Landry, Phys. Rev. E 66, 061303 (2002).
[33] J. Brujić, S.F. Edwards, D.V. Grinev, I. Hopkinson, D. Brujić, and H.A. Makse, Faraday Discuss. 123, 1 (2002).
[34] J. Brujic, S.F. Edwards, I. Hopkinson, and H.A. Makse, e-print cond-mat/0210136.
[35] J.W. Landry, G.S. Grest, and S.J. Plimpton, e-print cond-mat/0302115.
[36] G. Ovarlez, C. Fond, and E. Clément, e-print cond-mat/0212228.
[37] Y. Bertho, F. Giorgiutti-Dauphiné, and J.-P. Hulin, e-print cond-mat/0211510.


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