STRUCTURE OF GRANULAR PACKINGS

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Summary We report a numerical investigation of the structural properties of very large three-dimensional heaps of granular material produced by ballistic deposition from extended circular dropping areas. Very large heaps are found to contain three new geometrical characteristics not observed before: they may have two external angles of repose, an internal angle of repose, and four distinct packing fraction (density) regions. Such characteristics are shown to be directly correlated with the size of the dropping zone. In addition, we also describe how noise during the deposition affects the final heap structure.

Heaps of granular particles have been studied intensively during the past few decades both because of their great relevance for industrial applications and because, from a theoretical point of view, heaps are simple many-body systems well-suited to develop and probe theories [1, 2]. A major factor determining the pile structure is the force that it experiences during the deposition process. Lateral forces constraining 2D piles are quite different from lateral forces in 3D piles. So, it seems natural to investigate systematically the structure of *three-dimensional* packings subjected to more complex lateral forces and to see whether they imply hitherto unnoticed features. Although static piles of granular materials are classical examples of packings [5], to date there has been no systematic study of spatially resolved packing properties of 3D heaps. Three-dimensional packings require using a large number of particles, of the order of two to three orders of magnitude more than in 2D scenarios.
Here we report a study of the density distribution and the angle of repose measured for very large 3D heaps of monodisperse spherical particles. We report results obtained for heaps with up to 2.5×10^7 particles dropped sequentially onto a horizontal plane from a homogeneous "rain" of particles emerging from a circular area-source with adjustable radius. Three-dimensional simulations are hardly feasible with a full molecular dynamics approach but there are efficient alternative ways to address the problem. Here we use the well-known Visscher–Bolsterli (VB) algorithm [6, 7, 3, 4]. Particles follow the path of steepest descent until they stop after reaching either a local stable minimum or when touching the ground. After stopping, particles are not allowed to move anymore so that many-particle effects like, e.g. avalanches, cannot be simulated although a plethora of other effects are nicely reproduced [7, 3, 4]. The key advantage of the sequential VB algorithm is that it provides a realistic framework to rapidly compute the path of steepest descent and, therefore, allows us to investigate very large assemblies of particles, not accessible with other models. Of main interest is to determine bulk properties such as density, contact numbers, repose angles, etc.

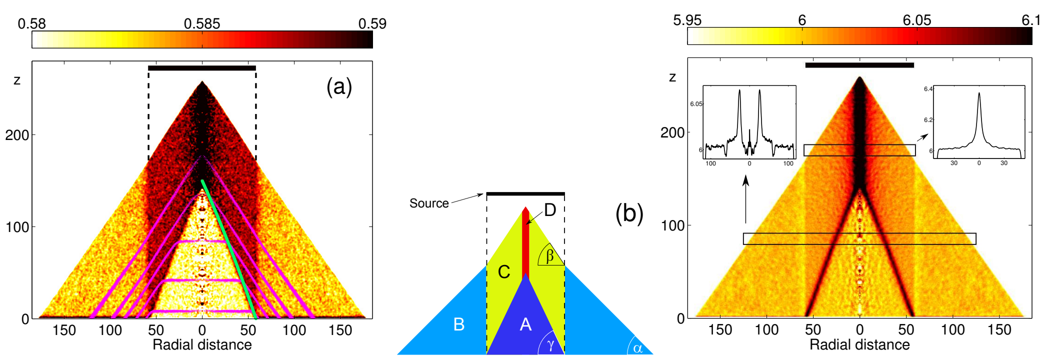

Figure 1. (a) Packing fraction for a heap with five contours superimposed showing the growth history and that the flat horizontal surface decreases as the growth proceeds. The green line segment on the right of the inner triangle shows the prediction of Eq. (1). Here $N = 10^7$. (b) Schematic representation of a generic heap structure and its main characteristics: the angles of repose α, β, γ, and the four characteristic density zones denoted by $A..D$. (c) The average contact numbers inside of the heap as a function from radial distance from the heap axis. The insets display the variation of contact numbers along the two rectangles, as indicated. Here $N = 10^7$.

Figure 1a shows the packing fraction as a function from the radial distance from the heap axis for a three-dimensional heap made of $N = 10^7$ particles deposited sequentially from random positions in the extended circular source whose section is indicated by the solid black bar. To illustrate the growth history of the pile, we superimposed to it five contours showing the evolving shape obtained after depositing $N = 10^5$, 5×10^5, 10^6, 1.6×10^6 and 3×10^6 particles. From these contours one sees how the inner triangular density cone gets formed as the flat horizontal surface gets smaller and smaller when the particle deposition proceeds. The packing fraction was obtained using cylindrical coordinates (r, z, ϕ) coaxial with the heap. For masses m_i with center of mass at $\mathbf{r}_i$ then we measured the density $\rho(r, z, \phi)$ at position $\mathbf{r}$ using the definition [8] $\rho(\mathbf{r}) \equiv \sum_i m_i \phi[\mathbf{r} - \mathbf{r}_i]$, where ϕ is a Gaussian coarse-graining function $\phi = \frac{1}{\pi w^2} e^{-(|\mathbf{r}|/w)^2}$, $w = 2R$, and R is the particle radius. By averaging $\rho(r, z, \phi)$ over ϕ we get the density $\bar{\rho}(r, z)$, the quantity color coded in Fig. 1a.

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How does the packing fraction vary along large heaps produced by extended sources? This may be recognized both from the real heap in Fig. 1a and from the summarizing sketch in Fig. 1b. In general, we find heaps to contain four distinct density (packing) regions: First, there is a triangular region A under the dropping zone. When A grows, particles may eventually move outside the "shadow" of the dropping source forming the packing zone B. Since in this zone the VB algorithm requires moving particles to always maintain contact with the heap, outside the shadow of the dropping zone there is a region B where the particles are arranged more regularly than in A, which grows on top of a randomly deposited initial layer. Next comes region C, an intermediary packing that is less regular than that of B but more regular than that of A. Finally, in D we find the highest density of the heap.

The distinct density zones described above have a remarkable implication for the angle of repose. Instead of the familiar single angle of repose, we find heaps in fact to display two external angles of repose along with an internal angle, the boundary between A and C in Fig. 1b. We find a larger angle of repose under the dropping zone, and the usual angle outside it. These angles were measured as follows. For every z_i, we located the points r_i defining the outermost surface points around the heap, plotting them as $r = r(z)$. Using bins with $\Delta r = 10$ particle diameters, we fitted a straight line through the points (r_i, z_i) for each bin obtaining the dependence of the local angle of repose θ with distance from the axis.

The average number of contacts among particles is a classic measure to characterize the packing structure of spheres [9]. Thus, we determined the average number of contacts in a similar way as described above for the density but, of course, replacing $\rho(\mathbf{r})$ by $c(\mathbf{r}) = (\sum_i c_i)/n$, where c_i and $\mathbf{r}_i$ are the number of contacts and position of particle i, and n is the total number of particles inside of the averaging volume. The result of such counting is given in Fig. 1c and is clearly consistent with our findings described above, in particular the geometrical picture summarized in Fig. 1b.

In addition to the four areas that appear in the packing fraction, the distribution of contact numbers in Fig. 1c shows two new features: a pronounced jump in contact numbers as one crosses the boundary from the density region A to C, and a dip between areas C and B. The boundary between A and C corresponds to a "transition zone" i.e. to the points where the flat surface observed in the earlier stages of the construction of the heap meets the tilted surface. This sharp transition zone corresponds to an area of high contact numbers where the surface curvature is high (see Fig. 1a) and therefore we assume the local surface curvature to be responsible for the changes in the average contact numbers. The local curvature can be determined from the surface $r(z)$ described above. This assumption is consistent with the peak in contact numbers near the axis (area D): close to the top of the heap the mean curvature becomes very high.

As a final result, we mention that the angles α, β, and γ are not independent from each other and derive a relation interconnecting them. During the initial phase of the growth the heap has a flat surface (see the five contours in Fig. 1a). Particles falling onto this flat surface stay on it, since only a quite negligible amount falls of the edge. Particles that fall onto the tilted surface form a layer of approximately constant thickness on the whole inclined surface. From these assumptions it is possible to obtain a differential equation for $r(h)$, the function describing how the radius of the flat surface shrinks as the height h grows with time

$$\frac{dr}{dh} = -\cot\gamma = -\frac{(r + h\cot\delta)^2 - S^2}{(r + h\cot\delta)^2 - r^2}\cot\delta, \tag{1}$$

where S is the radius of the dropping zone and, for simplicity, here we approximate $\delta = (\alpha + \beta)/2$. Of course, this equation is only physically meaningful as long as $r \geq 0$. The solution obtained by numerical integration for $S = 60$ is shown by the green line in Fig. 1a. Solving the equation for $h = 0$ we get $\gamma_0 \equiv \gamma(h = 0) = \arctan(2\tan\delta) = 71^o$. Note that Eq. (1) can be rescaled with respect to S in such a way that only r/S and h/S appear in it. This means that Eq. (1) is scale invariant and needs to be solved just once, because of the relation $r_S(h) = x r_{S/x}(h/x)$.

In conclusion, 3D heaps of granular matter proves to be quite revealing. As summarized in Fig. 1b, we find such heaps to be characterized by several new geometrical features: (i) two external angles of repose α and β; (ii) an internal angle of repose γ, and (iii) four distinct density (packing fraction) regions, A, B, C, D. This means that instead of just the familiar single angle of repose, heaps may in fact display two distinct angles of repose, a fact implying the existence of four characteristic density zones in the heap. As for the external and internal angles of repose, α and γ, we showed them to be interrelated according to Eq. (1), a relation that depends of the radius S of the dropping zone ("rain of particles"). We have also performed an experiment to investigate the impact of noise in the deposition. Such experiment indicated that the duality of the angle of repose may be washed out by moderate to strong noise during the deposition process.

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