Granular Matter (2012) 14:163–168
DOI 10.1007/s10035-012-0343-2

ORIGINAL PAPER

Evolution of solids fraction surfaces in tapping: simulation and dynamical systems analysis

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Received: 9 August 2011 / Published online: 17 March 2012

Abstract We report our findings on the evolution of solids fraction in a tapped system of inelastic, frictional spheres as a function of the applied acceleration obtained via discrete element simulations. Animations of the simulation data reveal the propagation of a wave initiated from the base that causes local rearrangements of the particles ultimately leading to the development of a dense microstructure. We also describe the analysis of dynamical models capable of predicting the simulated behavior, and advanced visualization techniques for revealing the dynamics.

Mathematics Subject Classification 35C07 · 35Q51 · 37N15

Electronic supplementary material The online version of this article (doi:10.1007/s10035-012-0343-2) contains supplementary material, which is available to authorized users.

A.D. Rosato, D. Blackmore and X. Tricoche were partially supported by NSF grant CMMI-1029809. Computational resources were obtained from the Open Science Grid (under the support of the National Science Foundation and US Department of Energy's Office of Science) and Engineering Computing at NJIT.

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Keywords Solids fraction evolution · Dynamical systems model · Density wave visualization · Discrete element simulation · Vertical tapping

1 Introduction

An intrinsic property of granular materials is that their density can vary greatly depending on handling and environmental conditions. This has important consequences in the industrial sector concerned with the processing of bulk solids for the production of particulate-based products in everyday use. Perhaps one of the most interesting phenomena is *density relaxation* [16]—a term used to describe the process by which a granular material increases its bulk density as a result of mechanical disturbances, such as continuous vibrations, tapping or shearing. Packaged bulk materials transported over long distances often become compacted, which usually is an impediment in subsequent handling procedures. Alternatively, an improvement in packing efficiency in the processing of granular materials is often desirable in reducing costs and in meeting consumer demands.

The phenomenon of density relaxation has historical roots in the literature on packing studies, which can be traced back to Kepler in 1611, who in a pioneering work on crystals, conjectured that the densest arrangement of spheres was fcc (the subject of a later numerical proof by Hales [13]). Hooke followed with an exploration of the packing arrangements of disks and spheres. Since then, there has been continual interest in the subject. Recent investigations (of which we list only a few) on density relaxation have involved computational approaches, theoretical models and physical experiments[1–3,9,10,16,18,24,25,29,30,34]. We remark that the study of waves in continuously vibrated granular systems has also been a topic of interest, as in [32] or the experiments of

Eshuis et al. [11] who developed a phase diagram delineating five physical regimes in a layer.

The work reported here follows our earlier findings [31], which suggested that the process by which the bulk density increases is the propagation of an ordering effect of the flat base up through the assembly as the system potential energy is reduced. In this paper, we report on the non-monotonic evolution of the density of a vertically tapped system of uniform, inelastic frictional spheres as a function of the tap displacement amplitude at a fixed frequency. The dynamics during the application of a single tap-relaxation cycle are also examined, where an upward propagating density wave is observed. This wave causes the local rearrangement of the particles that, after many taps, produces a dense packing. We note that lateral vibrations have also been shown to cause an increase in bulk density [21].

In the next section, a concise description of the numerical simulations is given followed by an extended presentation and interpretation of the results. We then briefly describe our recent dynamical paradigm for tapped systems [5,6] in conjunction with an approach, including visualization, that can predict the simulated behavior. Our goal is to develop—from the models—scaling parameters capable of characterizing density relaxation.

2 Description of simulation

We simulate via the soft-sphere discrete element method the behavior of an assembly of inelastic, frictional spheres of diameter d and mass m that is subjected to a series of taps of frequency f and displacement amplitude a. We intentionally selected mono-disperse spheres (as opposed to a distribution of sizes) to correspond to experiments in the literature and as a continuation of our recently reported work. The computational volume consists of an open-top rectangular parallelepiped with laterally periodic boundaries, a square base of length $w/d = 12$ and a plane floor of infinite mass. Momentum is transferred to the particles by the floor which imparts a half-sine pulse at a fixed frequency $f = 7.5\,\text{Hz}$ over a range of displacement amplitudes $0.2209 \leq a/d \leq 1.2148$ that correspond to dimensionless accelerations $1.0 \leq \Gamma \leq 5.5$, where $\Gamma \equiv a\omega^2/g$, $\omega = 2\pi f$ and g is the acceleration due to gravity. Each pulse is followed by a relaxation interval during which the assembly of particles is allowed to collapse to a state of zero kinetic energy. We remark that an exploration of the effect of frequency is currently underway, and forthcoming results will be reported soon.

The collision force models used are those of Walton and Braun [35] in which normal and tangential impulses are functions of an allowed overlap between particles, typically less than 1 % of the diameter in accordance with the behavior of real colliding spheres. Along the direction of the line connecting the centers of two impacting sphere, linear loading and unloading springs respectively corresponding to constants K_1 and K_2 are used (where $K_2 > K_1$), which yields a constant restitution coefficient given by $e = \sqrt{K_1/K_2}$. The value of K_1 was chosen so that no overlap exceeds 1 % of a particle diameter. In the tangential direction, a hysteretic model is employed [36] in which particle tangential stiffness diminishes with increasing surface displacement until full sliding takes place at the friction limit μ. Thus particles can rotate due to the transmission of tangential impulses.

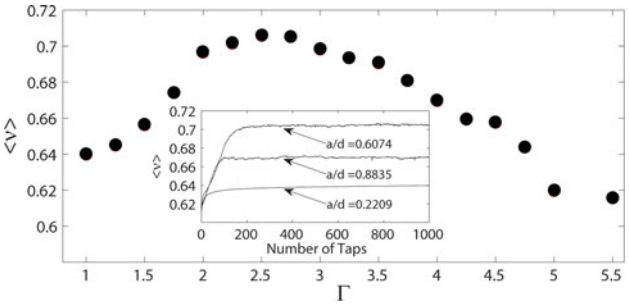

Fig. 1 The *black* disks are the ensemble-averaged solids fraction $\langle v \rangle$ as a function of acceleration Γ ($f = 7.5\,\text{Hz}$). Representative evolution *curves* of $\langle v \rangle$ for $\Gamma = 1, 2.75, 4.0$ are shown in the inset

Integration of the equations of motion through a time step $\Delta t \propto \sqrt{m/K_1}$, consequent on the loading period in the normal direction, is carried out with a Verlet algorithm. For the case studies reported here, acrylic particles are chosen having a mass density $\rho = 1200\,\text{kg/m}^3$, $e = 0.9$ and $\mu = 0.1$ in reasonably good agreement with the experimental measurements [19]. The integration time step was $O(10^{-6})$s. At $t = 0$, particles are randomly placed within the computational volume, and are then allowed to fall or pour under gravity until stable. An ensemble of 25 poured realizations was generated, such that the distributions of coordination number, solids fraction (mean value of $\langle v_0 \rangle = 0.609$) and free volume (as computed from Voronoi tessellations) were statistically indistinguishable.

The average solids fraction was monitored at the end of every tap-relaxation cycle and then an ensemble averaged value $\langle v \rangle$ was calculated over the realizations. An ample number of taps was completed so that the solids fraction temporal profile leveled out and this value was then selected as the steady state corresponding to the particular amplitude a/d under consideration. Results summarized in Fig. 1 show $\langle v \rangle$ as a function of Γ, while the insert presents typical evolution curves at $\Gamma = 4.0\,(a/d = 0.8335)$; $\Gamma = 2.75\,(a/d = 0.6074)$; and $\Gamma = 1.0\,(a/d = 0.2209)$. A non-monotonic dependence of the solids fraction on Γ is observed, which peaks around $\Gamma \approx 2.75$ where $\langle v \rangle \approx 0.709$ or approximately 95.6 % of the hexagonal close-packed value $\pi\sqrt{2}/3 = 0.7409$. The results also indicate that for large accelerations it is possible for the system density to be

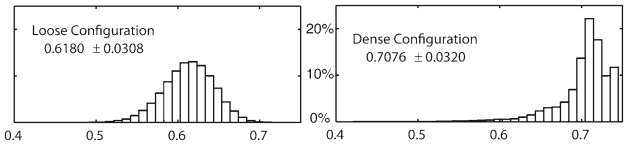

Fig. 2 Solids fraction (particle vol./Voronoi vol.) distribution of the poured system (ensemble averaged) and the assembly at $\Gamma = 2.75$, where $\langle v \rangle \approx 0.708$

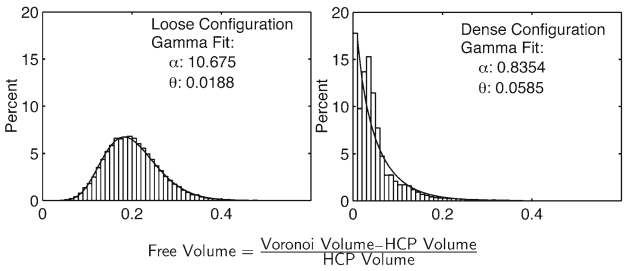

Fig. 3 *Top* Ensemble-averaged distribution of free volume for initial poured configuration. *Bottom* Distribution at $\Gamma = 2.75$, where $\langle v \rangle \cong 0.7076 \pm 0.0320$

reduced below the poured value. We comment that our maximum density corresponds to roughly a 16 % increase from $\langle v_0 \rangle = 0.609$, which is larger than that reported in [16] (approximately 9 %). We suggest that this discrepancy is due for the most part to the fill depth of our system ($\approx 22d$) as compared with the experiments ($\approx 435d$). Figure 2 provides comparison of the solids fraction distribution (via Voronoi diagrams) between the poured assembly (ensemble-averaged over 25 realizations) and at $\Gamma = 2.75$.

Evidence of the structural ordering at $\Gamma = 2.75$ is deduced from the free volume distribution (following [17]) $V_f = \left(V_{\text{poly}} - V_{\text{hcp}}\right) / V_{\text{hcp}}$, where V_{poly} is the Voronoi polyhedron volume and V_{hcp} is the same for a hexagonal closed-packing. Comparison of the distribution (Fig. 3) at $\Gamma = 2.75$ with that of the initial configuration (ensemble-averages over 25 realizations) indicates the development of a regular microstructure. Solid lines are fits[1] to the gamma distribution $f(x; \alpha, \theta) = \frac{x^{\alpha-1} e^{-x/\theta}}{\theta^{\alpha} \Gamma(\alpha)}$, where $\Gamma(a) = \int_0^{\infty} t^{\alpha-1} e^t \, dt$.

3 Dynamical systems model analysis

Here we describe the dynamical systems approach used to inform and complement the simulation and visualization aspects of our current research insofar as predicting behavior verifiable by comparisons and discovering general mathematical trends and relationships that might elude computational and visual investigation. The dynamical domain is $R := \{\mathbf{x} \in \mathbb{R}^3 : 0 \le x, y \le w, \ z_0(t; a, f) \le z\}$, where d is the diameter the particles, and z_0 represents the vertical tapping motion of the container floor, with $z_0(0; a, f) = 0$. The collection of particles is assumed monodisperse with a common diameter d and mass m. It is also assumed that the dynamics is periodic in the x and y so that one has periodic boundary conditions on the lateral boundaries of R. The particle centers are denoted by $\mathbf{x}_i = (x_i, y_i, z_i)$, which satisfy the properties: (i) There are N particles, $1 \le i \le N$; (ii) $0 < x_i, y_i < w$ for all i; and (iii) $z_0(t; a, f) < z_i$ for all i and $t \ge 0$. Finally, the interaction forces follow the Walton–Braun–Mindlin–Deresiewicz models described above.

It follows from Newton's 2nd law that the (vector) equations of motion can be written as

$$m\ddot{\mathbf{x}}_i = -mg\hat{\mathbf{e}}_3 + \mathbf{F}_i\left(\Delta\mathbf{x}(ij), \Delta\dot{\mathbf{x}}(ij)\right) \tag{1}$$

for all i, where $\hat{\mathbf{e}}_1$, $\hat{\mathbf{e}}_2$ and $\hat{\mathbf{e}}_3$ are the orthonormal basis vectors along the $x-$, $y-$ and z-axes, respectively, the dot denotes d/dt and $\Delta\mathbf{x}(ij)$ and $\Delta\dot{\mathbf{x}}(ij)$ represent the increments $\mathbf{x}_j - \mathbf{x}_i$ and $\dot{\mathbf{x}}_j - \dot{\mathbf{x}}_i$, respectively, for all nearest neighbors $\mathbf{x}_j$ of the particle at $\mathbf{x}_i$. One can solve (1) numerically, as our simulation does nearly optimally, but this is computationally expensive when N is very large and it is difficult to use the results for predictive analysis. Approximations of the mean-square displacements $\mathcal{D} := \sqrt{\sum_i \sum_j \left|\mathbf{x}_j - \mathbf{x}_i\right|^2}$, where $|\cdot|$ represents the usual euclidean norm, can be obtained as a function of time—a measure of the evolution of density.

Direct analysis of the system (1) to obtain even approximate solutions is nearly impossible for large N owing to the nonlinear nature of the $\mathbf{F}_i$. However, it is possible to prove, using techniques from the modern theory of dynamical systems [7,12,15,28], such qualitative results as *the system* (1) *exhibits chaotic dynamics if the amplitude a or the frequency f is sufficiently large*. But although this result and several others of a similar type can be verified rather routinely, detailed proofs would require considerably more space than is available in this paper. Given the difficulties inherent in the use of exact models, an important component of this research is to identify and exploit an approximate dynamical systems model that is simple enough to be amenable to extensive mathematical analysis, yet capable of effectively predicting much of the dynamics for a significant class of granular flows of current interest. In this regard, it is interesting to note that we have found in a work-in-progress [8] that by isolating the motion of the center of mass of a 1D configuration, we are able to obtain a rather simple model capable of indicating dynamical bifurcations of the complete system, very much along the lines of the method of averaging [15]. This, however, is a very special case that does not provide the kind of general model being sought.

One can treat (1) in the context of *lattice dynamics* [20,26,33,37], wherein it is assumed that the particles form a regular lattice (e.g., cubic), which automatically determines the nearest neighbors in (1) and allows to view the system

[1] Calculated using MATLAB 7.11 routine `gamfit` that generates maximum log-likelihood estimates of the parameters α and θ.

as differential difference equations that are all, except at the domain boundary, represented by a single equation. Then exact solutions—especially of the traveling wave kind—can sometimes be found by making an ansatz about the form of the solutions, as in [20,26,33]. This approach is most effective in 1D systems, but results such as those in [37] indicate that it can be extended to (1).

Another approach to (1) is to derive continuum (PDE) models using limiting processes, such that the resulting dynamics mimics that of the Newtonian system. One popular method is the *long wavelength limit* (*LWL*) in which the particles form a regular lattice with edge length h much smaller than any acoustic wavelength. The particle positions are expanded in Taylor series in h, and truncated at a convenient order (usually four) to produce PDEs for the coordinates, which in the case of (1) yields

$$(x, y, z)_{tt} - \nabla^2(\kappa_1 x, \kappa_2 y, \kappa_3 z) = (G_1, G_2, G_3), \tag{2}$$

where $\nabla^2 := \partial_\xi^2 + \partial_\eta^2 + \partial_\zeta^2$ is the Laplacian expressed in terms of the limit variables (ξ, η, ζ), the κ_i are positive constants and the G_i are nonlinear functions of the coordinates and their partial derivatives of order up to four. These limits have been studied for 1D configurations by several researchers including [6,14,22,23,27], and have been shown to be integrable (defined in [7,12]), with soliton solutions, in the ideal (isoenergetic) case [6,22]. In the 2D and 3D cases, it may still be possible to modify existing methods to show that (2) exhibits interesting wave dynamics. Observe that if one has a solution of (2) and the auxiliary conditions, it is easy to determine the evolution of the density using the continuity equation, which is of course of considerable importance in the study of granular flows.

The BSR method for generating approximate infinite-dimensional dynamical models for granular flows uses a locally averaged limit in the transport mode along trajectories as $N \to \infty$ to produce an integro-PDE of the form [4]

$$D_t \mathbf{u} = -g\hat{\mathbf{e}}_3 + \int_{\mathbb{R}^3} \Phi\left(\mathbf{y} - \mathbf{x}, \mathbf{u}(\mathbf{y}, t) - \mathbf{u}(\mathbf{x}, t)\right) d\mathbf{y}, \tag{3}$$

where $\mathbf{u}$ is the velocity, D_t is the total derivative and the kernel Φ vanishes outside a small neighborhood of $\mathbf{x}$. This model appears to be the most promising for a variety of reasons including the following: An investigation of this model in the 1D ideal case [5,6] has shown that this dynamical system is also integrable, and it appears that the same is true of higher dimensional versions. If the system is dissipative as we are assuming in this study, our preliminary research indicates that there is still a rather good chance of finding decaying traveling wave solutions. The left-hand side of (3) is just the general kinematic wave equation operator; hence, this equation should be (as strongly indicated in our investigations so far) well-suited to studying wave propagation and shocks via characteristic-based methods. Numerically speaking, (3) together with any associated auxiliary conditions also comprises a boundary value problem, but the lower order and integration lead to improved convergence over the LWL method. And as in the LWL, a solution of this model can be used to calculate the density.

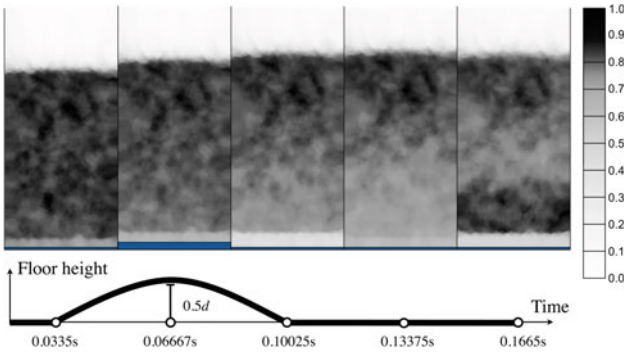

Fig. 4 Animation of evolution of $\bar{v}_{loc}$ at $\Gamma = 2.25$ ($f = 7.5$ Hz)

4 Visualization of dynamics

To better understand the physical mechanism, animations of the dynamics were completed. For this, we saved configurations (particle coordinate positions) every 10^{-5} s based on simulations of the wave speed in a granular column of the order of 150 m/s and the system fill height of $\approx 22d$.

The visual analysis of the resulting transient data focused on a continuous animation through which the dynamic evolution of the system could be monitored. Important visual cues about the spatial organization of the assembly were obtained through global illumination of the scene. The second part of our analysis focused on the quantitative study of the evolution of a relative solids fraction $\bar{v}_{loc} := v_{loc}/0.7409$, where v_{loc} is the local solids fraction. Specifically, the 3D Voronoi diagram of the particle set was constructed for each saved configuration to enable the assessment of the local solids fraction $v_{loc} := (\pi d^3)/6V_{\text{poly}}$, where V_{poly} is the volume of the encapsulating Voronoi polyhedron. These 3D diagrams were then mapped to 2D images by integrating along rays perpendicular to the tapping plane. This measure gives values in the interval (0, 1], whereby the wave itself corresponds at each step to a spatially coherent region of low values.

Figure 4 shows a sequence of frames taken from the animation [2] of $\bar{v}_{loc}$ at $\Gamma = 2.25$ for a single tap ($f = 7.5$ Hz) of duration 0.06667s followed by a relaxation period (floor is stationary) lasting 0.06667s. In the gray scale image, dark grey corresponds to the maximum $\bar{v}_{loc}$ attained ($\simeq 0.87$). Please refer to the provided scale in Fig. 4. The first frame at $t = 0.0335$s corresponds to the start of the wave pulse.

[2] See online supplementary material

From the evolution of $\bar{v}_{loc}$ in the animations, we observed the following sequence of events. At the outset, the system begins to translate en masse upwards and as a result of the transmission of impulses through particle contacts, dilation of the system commences. The second frame in the sequence is the map $\bar{v}_{loc}$ when the floor has reached its peak position, while the third frame is the configuration when the floor is at the zero position and has stopped moving. At this time, the assembly is still dilating ($t \approx 0.1s$). The expansion reaches a maximum dilation at $t \approx 0.13375$s (frame 4) after which particles on the average start to move back down.

When spheres near the bottom collide with the floor, they bounce slightly up thereby propagating some upward momentum to the particles that lie above them. The last frame in the figure shows $\bar{v}_{loc}$ at $t = 0.1665$s, where the shock can be seen moving upward shortly after the assembly has collided with the floor. Eventually, a density profile is locked in as the kinetic energy of the system decreases due to inelastic collisions. The application of continued taps in the same manner ultimately produces a system having a steady-state density ($\sim$0.70 at $\Gamma = 2.25$ in Fig. 1).

5 Summary and conclusions

A discrete element model was used to simulate the density relaxation in an assembly of uniform, inelastic, frictional, soft spheres within a laterally periodic box subjected to taps imposed by the motion of a flat plane floor. Material properties were selected to correspond to acrylic, the tap frequency was fixed at 7.5 Hz and a wide range of tap displacement amplitudes were chosen. We find a non-monotonic dependence of the ensemble-averaged bulk solids fraction (or equivalently bulk density) on dimensionless acceleration Γ, with a peak value that is approximately 95.6 % of the theoretical maximum value. There is an accompanying shift of the solids fraction distribution from an initially random structure to one that contains a significant degree of HCP order.

Animations of the evolution of normalized solids fraction revealed a process during a single tap whereby the assembly dilated, reaching a maximum after the floor motion had ceased. As particles begin to move downwards in a 'contraction process', collisions with the floor cause an upward propagation impulses that eventually locks in a density profile. Finally, analysis of the dynamical systems models for the relaxation flows yield predictions consistent with both the simulations and visualizations. Thus, the dynamical systems—simulation—visualization approach appears to be very promising for the investigation these granular flows.

Acknowledgments The authors thank O. Walton for insightful discussions.

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