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Molecular dynamics simulations of hard sphere granular particles

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We use molecular dynamics to study the two dimensional granular flow of particles that interact with each other via a hard sphere potential with inelastic collisions characterized by a coefficient of restitution. The particles are confined in a two dimensional box that contains a hole at the bottom through which particles flow under the influence of gravity. The particles develop coherent flow patterns that look similar to those seen in observations of real granular flow. The velocities of discharging particles through the hole is independent of the depth. We also study the fluidization of the granular particles that sets in when the bottom wall undergoes harmonic oscillation. The dense hard sphere gas is found to reproduce many of the unique features of the granular flow.

Granular particles (see, for example, ref. [1]) display challenging phenomena that have recently attracted considerable attention from the physics community [2–9]. Granular particles flow like liquid under certain conditions and exhibit interfacial instability [4–5]. But under different conditions, they endure stress and support themselves with a finite angle of repose [3–6]. In this case, they behave like a solid. Because of this dubious nature, we find a sharp departure in the gravitational flow patterns of the granular media in contrast to what is seen in a normal liquid. For example, consider the flow of sugar in a confined geometry, say a cup. We open a hole at the bottom and let sugar escape through the hole. The flow of sugar is different from that of a liquid in several respects. First, the velocities of the escaping particles are independent of the depth of the sugar in a cup. However, the discharge rate R at the hole, defined as $R = nAv$ with n the density of particles, A area and v the velocity, is a function of the hole size. It is reported that $R \approx a^{2.5}$ with a the radius of the

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hole[#1]. If it were a liquid, the velocities would be independent of the hole size but proportional to $h^{1/2}$ with h the depth. Second, the free surface of the sugar develops a kink at the center with the kink angle given by the angle of repose. Third, as time $t \to \infty$, not all the granular particles are discharged through the hole. There remain particles inside the cup that support themselves, while in the liquid case, all the particles eventually flow out (fig. 1). These are examples of most simple gravitational flow problems of granular particles in a confined geometry. Yet, as far as we know, there exists no continuum theory that satisfactorily explains even these most simple flow patterns (see, for example, ref. [10]).

In the absence of any analytic theory available at this moment, we thus find it particularly interesting to carry out computer simulations. The model used assumes that granular particles interact with each other via a hard sphere potential (or actually hard disk, since our simulations were two dimensional) with inelastic collisions allowed for through a coefficient of restitution[#2]. They move under the influence of gravity and interact only when they collide. Our model ignores other interactions among particles such as those caused by cohesion, humidity and/or electrostatic forces. We also neglect frictions among particles except that particles lose energy via inelastic collision. While there have been various proposals for the friction laws in the literature, we neglect them in this work except allowing particles to lose their energy via inelastic collisions and would like to see whether this simple model reproduces many of the unique features of the granular flow.

In this paper, we pay particular attention to the following problems. First, the evolution of the free surface and the flow patterns without an obstacle. Does a dense hard sphere gas exhibit peculiar granular flow patterns? Second, are the velocities of discharging particles independent of the depth as is seen in granular media? Do they obey the power law observed in real experiment? Third, fluidization of granular media when the bottom wall undergoes harmonic oscillation. Granular media can be fully fluidized and undergo significant volume expansion when the bottom wall is stirred. In particular, it has been reported that the granular media suddenly undergo a solid–liquid transition when the bottom wall is set to harmonic motion [5] (fig. 2). This is a quite interesting interfacial instability problem, yet there seems to be a long way to

[#1] Since the velocity is given by $(gh)^{1/2}$ for a liquid, a simple scaling argument yields that the velocity of the granular particle through the hole should be written as $v = (gh)^{1/2} G(a/h, D/a)$ with D the particle size. If we assume the experimental fact that v is independent of the depth, then the only way to satisfy this observation in the limit of $D/a \ll 1$, is to cancel the h dependence. This predicts $v \approx (ga)^{1/2}$, thus the flow rate $R \approx a^{5/2}$. Scaling, however, does not predict why v should be independent of the depth. In general, the velocity v for the granular particle should be written as $v = (ga)^{1/2} G(D/a)$.

[#2] A discrete model based on random walk was recently proposed. This model exhibits many of the unique features of the granular flows in a confined geometry. See ref. [11].

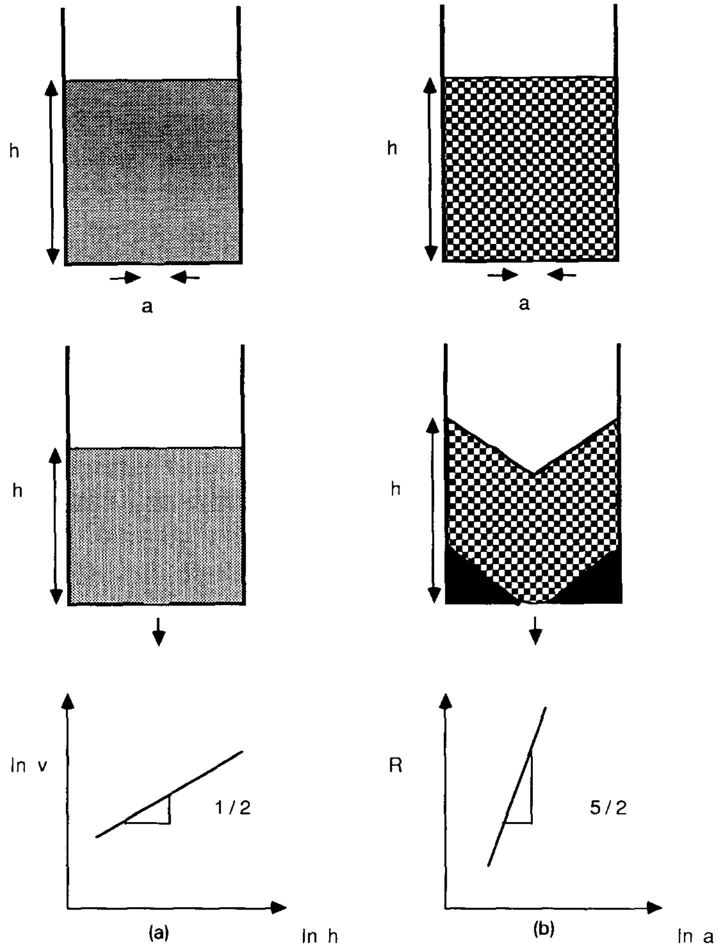


Fig. 1. Schematic description of different flow patterns of normal fluid (a) and granular media (b). For granular media, the free surface develops a kink and the velocity v of the outgoing particle is independent of the depth but depends on the radius of the hole a. Experiment indicates that the discharge rate $R = nvA$ with A area and n density of the particles is proportional to $a^{2.5}$ (see refs. [1, 10]). Moreover, as time $t \rightarrow \infty$, there remain particles inside the box (black region in (b)) that supports themselves with a finite angle of repose. On the other hand, for fluid, the free surface remains flat as fluid escapes through the hole and the velocity of the outing fluid is proportional to $h^{1/2}$. Also, there remains no fluid inside the cup as $t \rightarrow \infty$.

come up with a rigorous stability analysis. We present simulation results for the fluidization process associated with this oscillation.

The simulation method generally follows standard procedures of molecular dynamics for hard spheres (disks) [12]. The system consists of N disks with unit mass and diameter D, in a square box with side wall $L = 1$. In most of the runs we used $N = 900$, and D ranged from 0.02 to 0.03. For an isolated hard sphere or hard disk system, a quantity with dimension of time can be obtained only

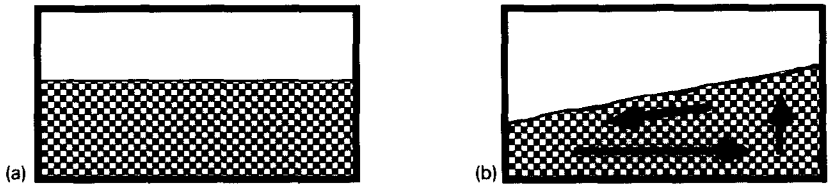


Fig. 2. Liquid–solid transition occurs for the granular media when the bottom wall undergoes harmonic oscillation (see ref. [4]). (a) Without oscillation; (b) with oscillation.

with use of the temperature; runs at different temperature differ only in time scale. In our simulations the temperature generally varies with time, but the initial temperature can be used to fix a time scale. Let τ be the time needed to traverse the box by an average particle at the initial temperature, $\tau = L(m/kT)^{1/2}$, where k is the Bolzmann constant. Generally our runs were the initial temperature $kT = 1$, and since $m = L = 1$, the time unit is $\tau = 1/\sqrt{2}$. In the following velocities and other rates are usually expressed in terms of this unit, but in some cases it is more convenient to use dimensionless variables. We consider processes taking place under gravity; a dimensionless parameter which measures the importance of gravitational vs. thermal effects is $\alpha = mgD/kT$ where g is the gravitational acceleration. In terms of the initial temperature, α had values covering a fairly wide range, from about 1 to about 3000.

Collisions were inelastic, with a coefficient of restitution ε; the relative velocity of two particles after a collision is reduced by the factor ε from the value it would have if the collision were elastic. Thus if $\boldsymbol{e}$ is the unit vector between two particles in contact and $\boldsymbol{v}$ is the initial relative velocity, then the relative velocity $\boldsymbol{v}'$ after the collision is given by $\boldsymbol{v}' = \varepsilon(\boldsymbol{v} - 2\boldsymbol{e}\,\boldsymbol{v}\cdot\boldsymbol{e})$. Values used for ε were about 0.95.

The disks were initially placed on a square lattice, with a Maxwellian distribution of velocities. They were then allowed to settle under the influence of gravity. After a few hundred-thousand collisions the bottom half or so of the system forms a triangular lattice, with density near the bottom within a few percent of the close-packing density $n_c = 2/(3D^4)^{1/2}$. The lattice is not perfect but shows defects such as vacancies and dislocations; however there is clear ordering through about 27 layers. The upper layers become more amorphous, and the top most particles lie about 85% of the way up the box (that is, the top 15% of the box is empty). Formation of the ordered region requires that the temperature be low enough; at high temperatures the system forms a gas. (This formation of a solid phase is different from that observed for an isolated hard sphere system, which is a purely density-dependent effect). For our purpose the formation of the solid phase is essential as one would not expect granular flow in a gas system. In the settling process gravitational energy is converted into kinetic, so there is heating which would prevent formation of the solid phase if the collisions were elastic; the inelastic collisions prevented such process being used for subsequent runs with various hole sizes.

We now turn our attention to the simulations results.

(*A*) *Evolution of free surface.* We first present real experimental data of granular flow patterns. The experiments were conducted at Lehigh with glass beads of radius 0.4 mm [#3]. The glass beads, initially confined in a two dimensional box of size $0.305\,\mathrm{m} \times 0.915\,\mathrm{m} \times 0.019\,\mathrm{m}$, were discharged through the hole at the bottom, with diameter about 1 cm. Fig. 3 shows snap shots of the evolving patterns of the free surface. Initially a small downward bump appears near the center line, which soon develops what appears to be a singular tip at the front. The front then moves downward while preserving its tip angle. When the tip reaches the bottom, the motion stops and the particles below the free surface are permanently trapped inside the box.

The goals of this simulation are to determine whether the hard sphere model produces what is observed in real granular flows regarding (i) the evolution of the free surface, (ii) the velocities of the discharging particles. The simulations were done for hole diameters ranging from 3 to 30 particle diameters.

The flow develops in several stages as follows. First, particles in a wedge, or triangular-shaped region (that is, an equilateral triangle with base corresponding to the hole), fall out under the influence of gravity. These particles fall almost freely; because of the uniform acceleration the lattice planes separate as they fall so particles in this region undergo few collisions. In contrast, particles elsewhere are nearly locked into a close-packed configuration and so are slow to develop any coherent flow velocity. As the wedge empties, a second stage develops during which particles near the boundaries of the wedge develop a flow downward and towards the hole. Eventually this flow pattern occupies most of the system. The flow has a roughly radial shape, but is not completely symmetrical, due to lack of complete symmetry in the initial configuration. If friction at the bottom wall is present, there are passive regions, with an upper boundary slanting down towards the hole, which do not partake in the flow pattern; in the absence of wall friction these regions have a flow pattern towards the hole. The velocity of particles passing through the hole increases linearly with time (with large fluctuations) during the first stage, then levels off and remains roughly constant (again, with large fluctuations) during the second stage. It is during this second stage that most ($\approx 70\%$) of the emptying takes place; this stage exhibits characteristics of granular flow. In the subsequent

[#3] We wish to thank H. Caram for providing these pictures.

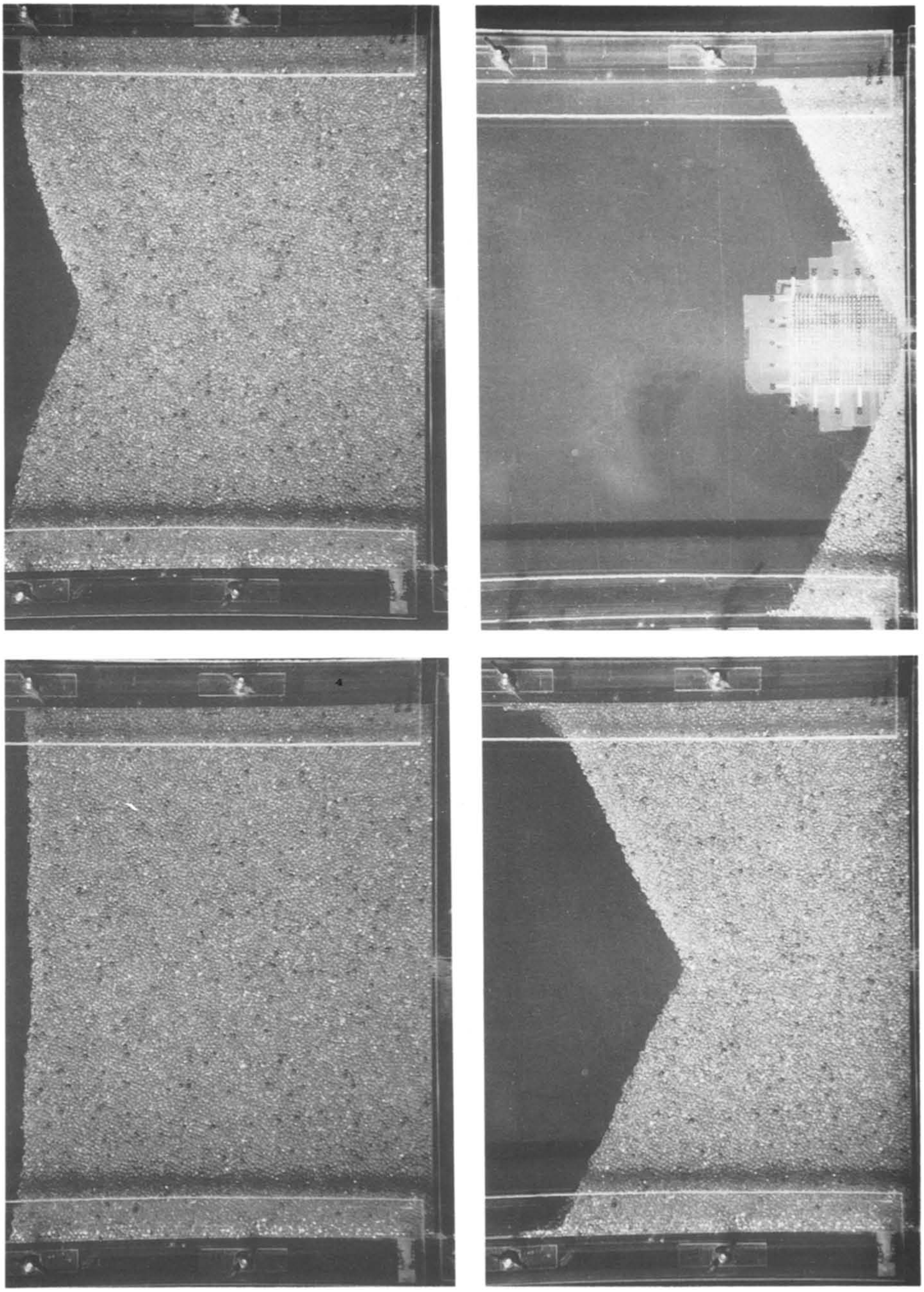


Fig. 3. Evolution of free surface of granular particles in a two dimensional rectangular box of size $0.35\ \mathrm{m} \times 0.915\ \mathrm{m} \times 0.019\ \mathrm{m}$. The diameter of glass beads used in this experiment is 0.6 mm.

final stage, the velocity of leaving particles drops and the system looks like a fluid. The development of a flow pattern is accompanied by significant changes in density and temperature. The density near the bottom drops fairly quickly from $\approx 95\%$ of close packing to $\approx 80\%$ when about 1/3 of the particles have been removed. The temperature changes more dramatically, increasing, depending on the conditions, by a factor of as much as several thousand over the same period. Corresponding to the increase in temperature, α (measured in a region lying directly above the hole, 5 diameters high) drops to a value of about 0.5; this value is fairly stable over large changes in the gravitational acceleration. Thus the time scale of the dynamics is determined by g rather than by the initial temperature.

When the hole size is small, an arch develops above the hole after a few particles are discharged (fig. 4). Once the arch is formed, a further discharge of the particles is prohibited and all the particles are permanently locked near their original positions. When we gently stir the bottom, then we can initiate the discharging process again. For the hole size 5, similar behavior was observed and thus the pictures are not displayed. Upon increasing the hole diameter, we can remove the arch and trigger the steady flow of particles through the hole. The snap shots of the flow patterns at different times are shown in fig. 5. We first allow the particles to settle down under the influence of gravity. After that, we open the hole at the center of the bottom. The flow patterns shown in fig. 5 are for the hole size $a = 10D$ and the total number of collisions that take place during the simulations is about 1.1 million, of which about 90% are usually binary collisions (the remaining 10% being collisions with a wall). Note that there appears a sharp boundary between the active regime and the passive regime, which defines the angle of repose in the literature. In our simulation, due to the formation of a regular lattice, however, this angle is given by 60°. This is larger than a reported experimentally observed value, 15–20° [3], but not far from our own experimental value

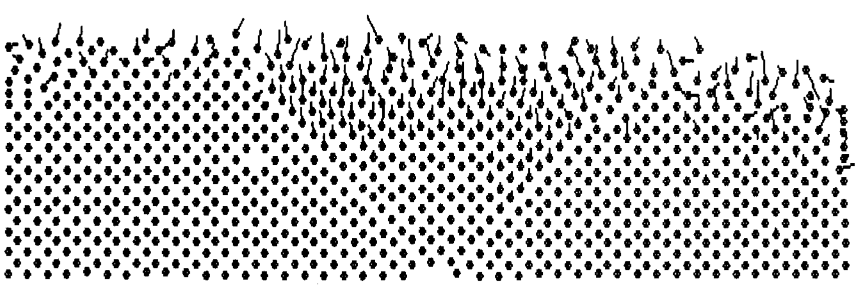


Fig. 4. Formation of an arch above the hole for the hole size $a = 3D$ with D the diameter of the particle.

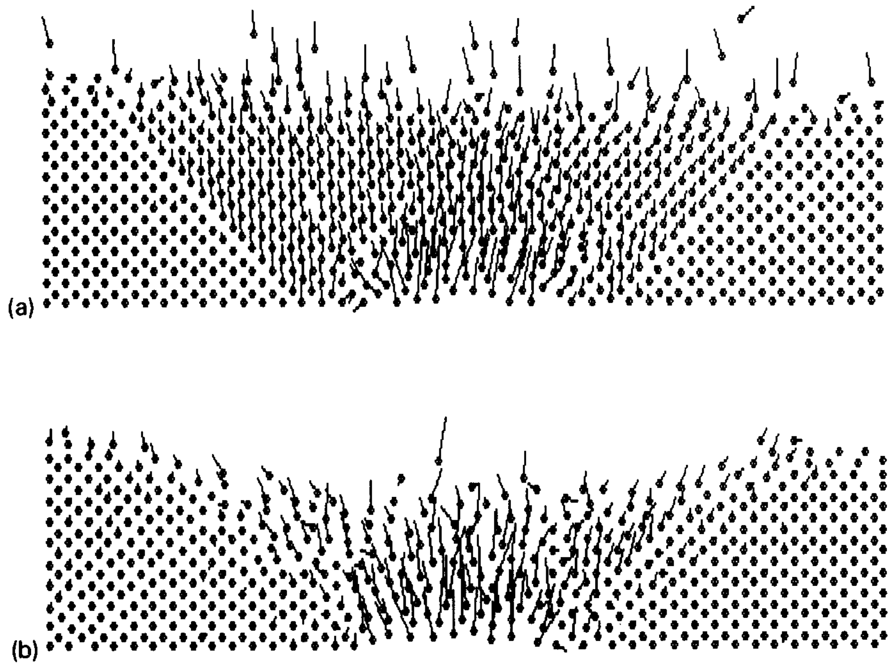


Fig. 5. Snap shots of the two dimensional molecular dynamics simulations of a very dense hard sphere particles. Initially, the particles are regularly spaced in a two dimensional box. The initial velocity distribution of the particles is Gaussian. The particles then undergo random collisions and fall along the vertical direction under the influence of gravity. Once they occupy approximately the half of the box, we open the hole at the bottom. Two sequential flow patterns with a hole size $a = 10D$ are shown in (a) and (b).

$\theta \approx 40°$. The main reason we obtain 60° for the angle of repose is because we started the simulations with a regular lattice. If we shoot particles randomly from the top or gently tilt the configuration to let the particles flow, one could easily monitor this angle by adjusting the coefficient of restitution f. Since one of the main purposes of this paper is to determine whether the hard sphere MD produces some of the experimentally observed flow patterns, we are encouraged to see that the simulation results produce flow patterns which are qualitatively similar to those observed in real granular experiment (fig. 3).

(B) *Velocity of the discharged particles through the hole.* In this part, we examine the velocity of the outgoing particles through the hole. As mentioned in the introduction, for granular flow the velocity is independent of the depth. In fig. 6 are shown the velocities of the outgoing particles as a function of time

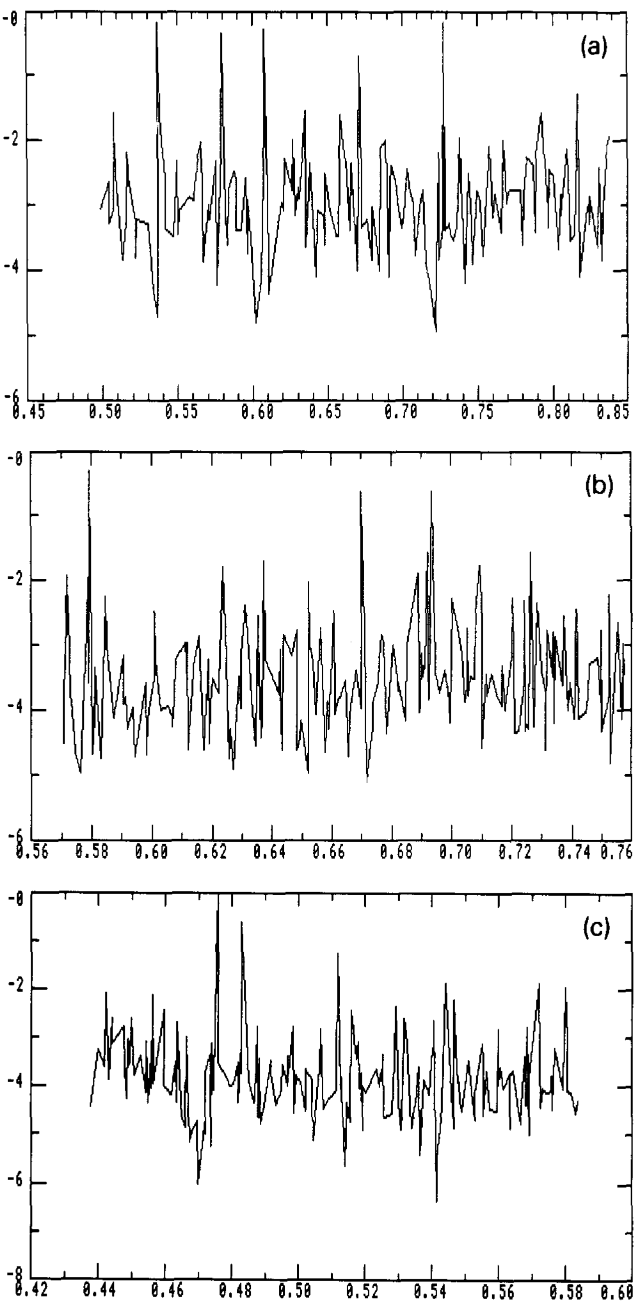


Fig. 6. Velocity of the outgoing particles as a function of time for the hole size $a = 7$ (a), 10 (b) and 12 (c) in units of D. The velocity fluctuates rapidly, but the mean value remains constant.

for the hole sizes 7, 10 and 12 in units of D. The velocity shows strong fluctuations but the mean velocity remains the same. This seems to be a rather strong confirmation that hard sphere gas is indeed a valid model for the granular particles. We do observe that the mean velocities slightly increase as the hole size increases. The mean velocities obtained by simulations are: $v = 3.2$, 3.6, 4.0 for the hole sizes $7D$, $10D$ and $12D$ respectively. It is, however, difficult to confirm the predicted 2.5 power law. It is because the ratio of the hole size to the box is too large in comparison to real experimental situations. Nevertheless, it is encouraging to see that the velocity is independent of the depth, which is one of the sharp departures of the granular particles from fluid flow.

(C) *Fluidization of granular particles.* Finally, we investigate the fluidization process of the granular particles. In a recent article, it has been reported that fluidization occurs when the bottom wall undergoes harmonic oscillation [4]. Under this condition, it has been argued that granular media become fluidized only when the maximum acceleration induced by the oscillation is greater than the gravitational acceleration. Let the amplitude of the oscillation be A and the frequency of oscillation be ω. In ref. [4] it is reported that De Gennes in his unpublished report proposed the criterion for the onset of fluidization:

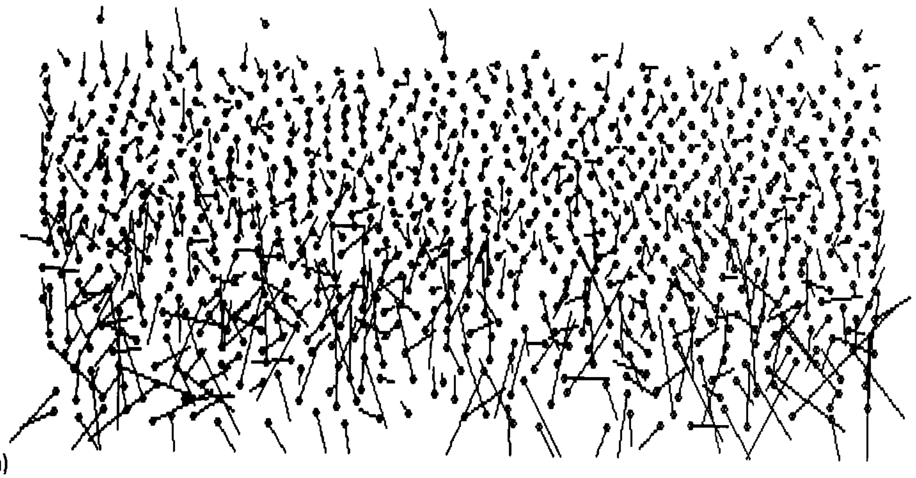
$$A\omega^2 > g\,.$$

This criterion is easy to understand. When external parameters such as the temperature and the diameter of the particles are fixed, then the only new length scale that enters the problem is $A\omega^2$. In order for the fluidization process to be initiated, the particle must be free to move upward against gravity. Thus $A\omega^2$ must be greater than g.

We have undertaken simulations to study the fluidization process of the granular media. We need some care to take into account oscillations in the simulations. In our simulations, the bottom wall undergoes periodic oscillation but remains stationary. In other words, it does not move but transfers momentum with an assigned frequency and amplitude whenever the particle hits the wall.

Let us first examine the length and the time scales of the system. The collision rate $1/\tau_c$ per particle in our simulations is of order of 10^2 to 10^3 (mostly 300–800). In order for the wall oscillation to have an impact upon the motion of the particle, the oscillation frequency ω must be smaller than $1/\tau_c$. If $\omega \gg 1/\tau_c$, then we expect that the oscillation merely introduces a random noise into the system and the coherent motion among granular particles would not be present. Next, assuming that the criterion proposed by De Gennes to be true, we expect the amplitude of the oscillation A to be larger than g/ω^2. We choose $\omega = 50$, $g = 40$ and thus $A \geqq 0.016$. We choose $A = 2D$ with D the disk diameter. The simulation results with a set of parameters are given in fig. 7a.

When $\omega \gg 1/\tau_c$ with $A\omega^2 \gg g$, the granular media becomes completely



(a)

(b)

Fig. 7. (a) Fluidization of granular particles for $\omega \gg 1/\tau_c$, when the bottom wall undergoes harmonic oscillation. The parameters in this run are: $\omega = 3000$, $A = 0.2D$. Initial temperature $T_i = 1.403$ up after 30 000 collisions to $T_f = 4.4795$. $\varepsilon = 0.97$ and $1/\tau = 332$. (b) Fluidization of granular particles in the opposite limit $\omega \ll 1/\tau_c$. $\omega = 22$, $A = 11.5D$. Initial temperature $T_i = 3.10$ goes up to $T_f = 7.327$ after 150 000 collisions. $\varepsilon = 0.97$ and $1/\tau = 279$.

fluidized and the volume indeed expands. In fig. 7 are shown snap shots of the simulation results for $\omega = 3000$, $A = 0.1D$, with hole size $a = 5$ at $T = 1.4$. The volume expansion is about 15% and the particles behave like fluids (fig. 7a). We, however, do not see any coherent motion develop inside the box as was observed in ref. [4]. In the opposite limit, $\omega \ll 1/\tau_c$ and $A\omega^2 \gg g$, we still do not see the appearance of a skewed surface as is seen in ref. [4], although the system becomes completely fluidized (fig. 7b). We carried out simulations for different sets of parameters that satisfy De Gennes' criterion. However, at this stage, we were unable to observe the onset of instability reported in ref. [4]. Moreover, a new discovery of our simulation is that within the context of our model, one may need an additional criterion other than the one proposed by De Gennes. There are two ways of satisfying the De Gennes criterion: i.e. fix the amplitude and increase the oscillation frequency, or fix the oscillation frequency and increase the amplitude. Our simulation results indicate that they do not appear to be the same. It seems to us that the oscillation frequency must be less than the collision rate in order for instability to set in. It is possible that the three dimensional nature of the flow as well as the friction among particles, which are absent in our simulations, may be important to initiate the instability. It is also equally possible that our modeling of oscillation might not be realistic.

In summary, molecular dynamics simulations of a very dense hard sphere gas appear to indicate that it is indeed a good candidate for modeling the gravitational flow patterns in slow limit. In particular, we found that the velocities of discharging particles through the hole are independent of the depth. However, we find that a further study is required to confirm the $a^{2.5}$ power law dependence as well as the onset of instability when the bottom wall undergoes harmonic oscillation.

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