Fluidization of a vertically oscillated shallow granular layer

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Molecular dynamics simulations are used to study fluidization of a vertically vibrated, three-dimensional shallow granular layer. As the container acceleration is increased above \( g \), the granular temperature and root mean square particle displacement increase, gradually fluidizing the layer. For nearly elastic particles, or low shaking frequencies, or small layer depths, the end of the fluidization process is marked by an abrupt increase in the granular temperature and rms particle displacement. The layer is then fully fluidized since macroscopic, fluid-like phenomena such as convection rolls and surface waves are observed. Increasing the total dissipation (by either decreasing the restitution coefficient or increasing the total number of particles) decreases the increase in granular temperature and rms particle displacement at fluidization, and shifts the increase to higher accelerations. Increasing the frequency also decreases the magnitude of the jump, and shifts the change to lower accelerations.

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I. NOTE FROM AUTHORS

After further investigations, we find that the results for the temperature and rms displacement at low \( \Gamma \) depend on the functional form of the velocity dependence of the restitution coefficient. Changing the dependence from \( e = \max\{e_0, 1 - (1 - e_0)(v_n/\sqrt{gd})^{3/4}\} \) to \( e = \max\{e_0, 1 - (1 - e_0)(v_n/\sqrt{gd})^{1/5}\} \) significantly reduces both \( T_{kin} \) and \( \Delta r_{rms} \) at low \( \Gamma \). The event-driven algorithm used in the present work has been tested and found to work well for situations where most collisions occur at high velocities, but this algorithm is less accurate for situations where many collisions occur at low velocities, as in the present work. Hence the results we have presented should be checked with an model that is more accurate for low velocity collisions.

II. INTRODUCTION

Granular materials are collections of many dissipative particles, which can behave as either a solid or a fluid [3]. To maintain a fluid-like state, energy must be continually supplied to the grains since it is dissipated during collisions. Often this energy input is realized by shaking a container vertically; the non-dimensional shaking acceleration is given by \( \Gamma = 4\pi^2Af^2/g \), where \( g \) is the acceleration due to gravity, \( A \) the shaking amplitude, and \( f \) the shaking frequency. With increasing \( \Gamma \) the behavior of the granular layer changes from solid-like to fluid-like. This fluidization does not occur abruptly at a particular \( \Gamma \) but rather is a process that develops over a range in \( \Gamma \). Even for \( \Gamma < 1 \), there is relative motion of the particles [2, 8], and the contact forces between particles show rich dynamics [4]. As \( \Gamma \) is increased above unity, the particles start to move randomly on length scales small compared to their diameter. This has been measured with laser speckle methods, where it was also found that in deep layers, upper layers fluidize first and then the fluidization proceeds downward [5] with increasing \( \Gamma \). The onset of macroscopically visible motion occurs at \( \Gamma \approx 2 \), depending on the experimental conditions [6].

Quasi two-dimensional geometries allow the study of the fluidization of vertically vibrated layers using direct imaging. Studies of horizontal monolayers have examined crystallization [7] and the coexistence of different phases that occur during fluidization [8, 9, 10, 11, 12]. In a vertical, initially crystalline layer a distinct jump in the height of the center of mass of the particles was found as the layer fluidized [13].

We present here results from fully three-dimensional molecular dynamics simulations of a shallow granular layer. The process of fluidization is accompanied by a smooth increase in temperature and particle mean square displacement that culminates in an abrupt increase for high coefficient of restitution, or low shaking frequency, or small layer depth. We identify this abrupt change with the end of the fluidization process.

III. MOLECULAR DYNAMICS SIMULATION

The event driven molecular dynamics simulation described in [14] was used for this study. The number of frictional, rotational spheres of diameter \( d \) used was varied to determine the dependence of fluidization on the layer depth, \( N \). The total number of particles was \( N \times 248 \), corresponding to a volume fraction of 0.58 at rest. The container was a box \( 15d \times 15d \times 300d \), in the \( x,y, \) and \( z \) directions, respectively, with the \( z \) direction being opposite to gravity. The bottom plate oscillated sinusoidally, \( z_\nu = A \sin(2\pi ft) \). The non-dimensional frequency, \( f^* = f \sqrt{Nd/g} \), was varied from 0.08 to 0.25. Unless otherwise noted, periodic boundary conditions were imposed in the \( x \) and \( y \) directions to avoid convection induced by frictional sidewalls [13, 16, 17, 18]. Surface waves were prevented from forming by choosing the horizontal dimensions (15\( d \)) to be smaller than the pattern.
wavelength, which was found to be $39d$ in simulations in a large box for a layer with depth $N = 3.6$, frequency $f^* = 0.15$, and $\Gamma = 2.3$.

The parameters characterizing the particles are the coefficient of normal restitution $e$ (the ratio of the relative normal velocity after collision to that velocity before collision), the coefficient of friction $\mu$, and the tangential restitution $\beta$, which gives the change in the relative surface velocity \cite{14, 19}. For this study, $\mu$ and $\beta$ were fixed at $\mu = 0.5$ and $\beta = 0.35$, which were the values used to reproduce surface wave patterns observed experimentally in oscillated layers of lead spheres \cite{14}. The normal restitution $e$ depended upon the relative normal velocity, $v_n$, of the colliding particles according to: $e = \max[e_0, 1 - (1 - e_0)(v_n/\sqrt{gd})^{3/4}]$, as in \cite{14}. The minimum value of $e$, $e_0$, was varied from 0.98 to 0.65.

Simulations were started from random initial conditions at $\Gamma = 3$. After 300 plate oscillation cycles, $\Gamma$ was reduced by 0.02. Particle positions and velocities were recorded at the phase where the plate was at its mean position and moving upwards. This procedure was repeated with $\Gamma$ decreasing by 0.02 each time until the particle collisions became too frequent for the event-driven algorithm to be usable \cite{20}. This limited our investigations to $\Gamma \gtrsim 1.6$, but we found that the accessible range in $\Gamma$ included the transition to full fluidization.

IV. RESULTS

A. Fluidization

The horizontal granular temperature $T_{kin}$, is the kinetic energy of the relative random motion of the particles,

$$T_{kin} = \frac{\langle (v_x - \langle v_x \rangle)^2 \rangle + \langle (v_y - \langle v_y \rangle)^2 \rangle}{2gd},$$  \hspace{1cm} (1)

where the averages are taken over all the particles and $T_{kin}$ has been made nondimensional by dividing it by the gravitational potential energy of a single particle raised by a height equal to its diameter. The averages are taken only in a horizontal plane to minimize the influence of the vertical shock wave \cite{21}. An example of the dependence of $T_{kin}$ on $\Gamma$ is shown in Fig. 1(a). A sharp increase in $T_{kin}$ is evident in the range $1.94 < \Gamma < 1.955$.

We compare $T_{kin}$ with the root mean square displacement,

$$\Delta r_{rms}(t) = \sqrt{\frac{\langle (x(t) - x(0))^2 + (y(t) - y(0))^2 \rangle}{d}},$$ \hspace{1cm} (2)

where $x(t)$ and $y(t)$ are the $x$ and $y$ positions of a particle at time $t$. To minimize the impact of particles crossing the periodic boundary on the measurement, the average is computed over all particles at least $5d$ from the boundary at $t = 0$. The rms displacement for $\Delta t = 1$ cycle(Fig. 1(b)) exhibits an increase at $\Gamma_f$, just as found for $T_{kin}$ (Fig 1(a)).

We define as fluidization the process that begins when $\Gamma < 1$ and ends at $\Gamma_f$, the acceleration where the abrupt increase in $T_{kin}$ and $\Delta r_{rms}$ occurs. After the increase, the layer is defined as vibrofluidized. This transition is history independent and non-hysteretic: it occurs at the same $\Gamma$ whether decreasing $\Gamma$ from 3.00 or increasing from 1.84, for step sizes that were as small as 0.01.

The granular temperature and density of vertically oscillated layers depend on the phase of the plate oscillation because, after each impact of the layer with the plate, a shock propagates upward through the layer \cite{21}. The phase dependence of $T_{kin}$ and $\Delta r_{rms}$ was examined for twenty equally spaced phases throughout a cycle, and all but one phase were found to yield similar behavior (Fig. 2). The one phase that yielded a different dependence on $\Gamma$ is labeled 4 in Fig. 2 at this point in the cycle the plate is near its minimum height and moving upward, which is where the shock has the greatest effect \cite{21}. However, the shock quickly travels through the layer, and its effects are negligible for most of the cycle. We therefore recorded data at the phase when the plate was at its mean position and moving upward.

Just as the vertical forcing may add a dependence on the phase of the driving cycle, it also creates gradients in the $z$ direction. The top layers are more fluidized than the lower layers, as Fig. 3 illustrates. While the fluidization process proceeds more rapidly for the topmost
layers, it does not complete until all layers have fluidized \( \approx N \). Similar behavior was found for \( f^* = 0.25 \).

B. Dependence on System Parameters

Changing the normal restitution coefficient has a dramatic effect on the granular temperature and rms displacement, as shown in Fig. 1. The transition to the fully fluidized state is most pronounced for our highest restitution value, \( e_0 = 0.98 \), and becomes less obvious as \( e_0 \) is decreased; for the lowest restitution value examined, \( e_0 = 0.65 \), no transition is discernible. As \( e_0 \) is decreased, the fully fluidized state is reached at higher \( \Gamma \): for \( e_0 = 0.98 \), \( \Gamma_f = 1.95 \); for \( e_0 = 0.85 \), \( \Gamma_f \approx 2.3 \).

The dependence of \( \Delta r_{rms} \) on \( \Gamma \) and \( e_0 \) is compared for three frequencies in Fig. 5. Increasing the frequency makes the fluidization process more gradual and decreases \( \Gamma_f \). For example, for \( f^* = 0.08 \) (with \( e_0 = 0.98 \)), \( \Gamma_f = 2.0 \), while if \( f^* \) is increased to 0.25, \( \Gamma_f = 1.85 \).

Increasing the layer depth leads to a less pronounced increase in \( T_{kin} \) and \( \Delta r_{rms} \), and the increase is shifted to higher \( \Gamma \) (Fig. 6). For \( N = 1.8 \), the end of the fluidization process occurs at \( \Gamma_f = 1.48 \), while for \( N = 5.4 \) the change is smaller and \( \Gamma_f \approx 2 \). Thus, as the total dissipation of the system increases, either by decreasing the restitution coefficient or by increasing the number of collisions (by adding more particles), the change from the fluidizing to the fluidized state becomes less pronounced and \( \Gamma_f \) increases.

After the layer has completed the fluidization process, fluid-like phenomena appear in addition to the increases in \( T_{kin} \) and \( \Delta r_{rms} \). For example, as is well known, surface waves appear at \( \Gamma \approx 3 \). We have done some simulations in a container large enough to accommodate waves and have found that waves emerge in a thin layer at about \( \Gamma_f \), while for a deeper layer, pattern onset occurs for \( \Gamma > \Gamma_f \) (see Table I). Additional simulations were made for a container with solid frictional lateral walls, and a single convection roll was found to develop at \( \Gamma = 2.24 \), the same \( \Gamma \) at which the fluidization process completes (Table I).

C. Comparison with Experiment

Comparing these simulations to experiment is problematic. Measurements of the granular temperature or rms displacement in a three-dimensional experiment are challenging since the trajectories of the grains in the bulk of the layer can not be recorded with just a simple video camera. Recently speckle visibility has been developed

| Phenomenon | \( \Gamma_{onset} \) | \( \Gamma_f \) | \( x \times y \) | \( e_0 \) | \( N \) | \( f^* \) |
|------------|-----------------|--------------|----------------|---------|-------|--------|
| Waves      | \( \approx 2.3 \) | 1.95         | 30 \times 30    | 0.98    | 3.6   | 0.22   |
| Waves      | \( \approx 2.3 \) | 2.3          | 30 \times 30    | 0.85    | 3.6   | 0.15   |
| Convection | 2.24            | 15 \times 15 | 0.95            | 3.6     | 0.15  |

FIG. 2: Phase dependence of the (a) granular temperature and (b) root mean square particle displacement in one cycle as a function of \( \Gamma \). The inset in (b) shows the height of the plate (normalized by the oscillation amplitude), \( z_P/A \), as a function of the phase \( \tau_f \) of the driving cycle. The temperature curves for different phases in the cycle are similar except for phase four (open triangles), which is influenced by the shock wave that passes through the layer after the particles hit the plate \([21]\). Filled circles indicate the phase used for the data presented in other figures. Simulation parameters were \( e_0 = 0.98 \), \( N = 3.6 \), and \( f^* = 0.15 \).

FIG. 3: Height dependence of (a) \( T_{kin} \) and (b) \( \Delta r_{rms} \), as functions of \( \Gamma \), measured above the surface of the plate. Fluidization completes at the same value of \( \Gamma \) for each height, but particles higher in the container are more mobile at lower \( \Gamma \). Here \( e_0 = 0.98 \), \( N = 3.6 \), and \( f^* = 0.15 \).
to measure the granular temperature in a 3D sample \[24\] and should be utilized to fully explore this process.

Umbanhowar and Swinney investigated the transition to surface waves for systems with similar layer depths and frequency using the pressure exerted by the layer on the bottom plate. They therefore recorded data at a different point in the driving cycle than was used in this work. In addition, the fluidization process may have completed at a lower \( \Gamma \) value than they report for the pattern transition as in our own work (Table I) \[22\].

Two groups have studied fluidization in deep layers \( (N = 15d \text{ in } [6] \text{ and } N > 20d \text{ in } [5]) \) and have reported that the fluidization of the layer begins at the top and proceeds downward as \( \Gamma \) is increased. Evidence of this top down fluidization can be seen in Fig. 3. Particles higher in the container are in a more fluidized, but fluidization is completed at the same value of \( \Gamma \) for particles at all heights studied.

V. DISCUSSION

We have shown that in shallow layers of nearly elastic particles, abrupt increases of both the granular temperature and the root mean square displacement indicate that the process of fluidization is completed. If the dissipation in the system is increased by adding more particles or decreasing the coefficient of restitution, the increases in granular temperature and rms displacement at full fluidization become more and more gradual.

While the granular temperature and root mean square displacement are good indicators of the onset of the vibrofluidized state, the question remains if there exists a single control parameter for the fluidization of a vertically oscillated granular sample. The non-dimensional acceleration \( \Gamma \) is not satisfactory since layers with different characteristics fluidize at different values of \( \Gamma \). The value of the temperature \( T_{\text{kin}} \) depends on the phase of the cycle, and both the rms displacement and \( T_{\text{kin}} \) at the onset of the vibrofluidized state depend on granular parameters such as coefficient of restitution and layer depth. Thus they do not make good measures. Others have suggested \( v_0 = A(2\pi f) \), but this measure does not collapse our data since we find a different dependence on \( f^* \) than that reported in [13]. We hope that our results will inspire further work on the process of fluidization in three-dimensional granular layers.

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![FIG. 4: (a) Linear and (b) logarithmic plots of the granular temperature, and (c) root mean square displacement as a function of \( \Gamma \) for different values of the normal restitution coefficient. The fluidization of the layer is more abrupt for particles that are nearly elastic. Simulation parameters were \( f^* = 0.15 \) and \( N = 3.6 \).](image)

![FIG. 5: The effect of varying the frequency on the \( \Gamma \) dependence of \( \Delta r_{\text{rms}} \). The change signaling the end of the fluidization process becomes more pronounced as the frequency is decreased. Here \( N = 3.6 \).](image)
FIG. 6: The effect of varying the layer depth $N$ on the $\Gamma$ dependence of $T_{kin}$ and $\Delta r_{rms}$. As the layer becomes thicker, the change signaling the end of the fluidization process becomes less pronounced. Simulation parameters were $f^* = 0.25$ and $c_0 = 0.98$.

[1] H. M. Jaeger, S. R. Nagel, and R. P. Behringer, Rev. Mod. Phys. 68, 1259 (1996).
[2] T. Pöschel, T. Schwager, and C. Salueña, Phys. Rev. E 62, 1361 (2000).
[3] S. Renard, T. Schwager, T. Pöschel, and C. Salueña, Eur. Phys. J. E 4, 233 (2001).
[4] P. Umbanhowar and M. van Hecke, Phys. Rev. E 72, 030301(R) (2005).
[5] K. Kim, J. J. Park, J. K. Moon, H. K. Kim, and H. K. Pak, J. Kor. Phys. Soc. 40, 983 (2002).
[6] N. Mujica and F. Melo, Phys. Rev. Lett. 80, 5121 (1998).
[7] P. M. Reis, R. A. Ingale, and M. D. Shattuck, Phys. Rev. Lett. 96 (2006).
[8] J. Olafsen and J. Urbach, Phys. Rev. Lett. 95, 098002 (2005).
[9] A. Prevost, P. Melby, D. Egolf, and J. Urbach, Phys. Rev. E 70, 050301 (R) (2004).
[10] J. S. Olafsen and J. S. Urbach, Phys. Rev. Lett. 81, 4369 (1998).
[11] A. Götzendorfer, J. Kreft, C. A. Kruelle, and I. Rehberg, Phys. Rev. Lett. 95, 135704 (2005).
[12] X. Nie, E. Ben-Naim, and S. Y. Chen, Europhys. Lett. 51, 679 (2000).
[13] A. Götzendorfer, C.-H. Tai, C. A. Kruelle, I. Rehberg, and S.-S. Hsiau, Phys. Rev. E 74 (2006).
[14] C. Bizon, M. Shattuck, J. Swift, W. McCormick, and H. Swinney, Phys. Rev. Lett. 80, 57 (1998).
[15] J. Talbot and P. Viot, Phys. Rev. Lett. 89, 064301 (2002).
[16] J. B. Knight, H. M. Jaeger, and S. R. Nagel, Phys. Rev. Lett. 70, 3728 (1993).
[17] J. B. Knight, E. E. Ehrichs, V. Y. Kuperman, J. K. Flint, H. M. Jaeger, and S. R. Nagel, Phys. Rev. E 54, 5726 (1996).
[18] R. D. Wildman, J. M. Huntley, and D. J. Parker, Phys. Rev. Lett. 86, 3304 (2001).
[19] O. Walton, in Particulate Two-Phase Flow, edited by M. Roco (Butterworth-Heinemann, Boston, 1993), p. 884.
[20] S. Luding and S. McNamara, Granular Matter 1, 113 (1998).
[21] J. Bougie, S. J. Moon, J. B. Swift, and H. L. Swinney, Phys. Rev. E 66, 051301 (2002).
[22] P. B. Umbanhowar and H. L. Swinney, Physica A 288, 344 (2000).
[23] F. Melo, P. Umbanhowar, and H. L. Swinney, Phys. Rev. Lett. 72, 172 (1994).
[24] P. K. Dixon and D. J. Durian, Phys. Rev. Lett. 90, 184302 (2003).
