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LETTER TO THE EDITOR

Heap formation in two-dimensional granular media

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Abstract. Using molecular dynamics (MD) simulations, we find the formation of a heap in a system of granular particles contained in a box with oscillating bottom and sidewalls. The simulation includes the effect of static friction, which is found to be crucial in maintaining a stable heap. We also find another mechanism for heap formation in systems under constant vertical shear. In both systems, heaps are formed due to a net downward shear by the sidewalls. We discuss the origin of net downward shear for the vibration-induced heap.

Systems of granular particles (e.g. sand) exhibit many interesting phenomena, such as segregation under vibration or shear, density waves in the outflow through hoppers, and probably most strikingly, the formation of heap and convection cells under vibration [1–4]. It has been known for more than one hundred years that granular particles on the top of a vibrating surface will form convection cells and heaps [5]. However, even with many recent studies on the subject [6–11], the exact mechanism for the heap formation is not established.

Recently, two experimental groups, Evesque *et al* [6] and Laroche *et al* [7] studied behaviours of granular particles contained in a box, while the whole box is being vertically vibrated. They confirm the formation of convection cell and heap. On the other hand, Zik *et al* find convection but no heap [8]. When viewed from above, these boxes are essentially squares, making the system fundamentally three-dimensional. On the other hand, there are some studies in two dimensions (i.e. a line when viewed from above) with fruitful results. Using molecular dynamics (MD) simulations of granular particles, Taguchi [9] and Gallas *et al* [10] found convection cells under vibration in two dimensions. Furthermore, they established the fact that the sidewalls are *inducing* the convection. However, the exact mechanism of how the convection is induced by the wall is still not firmly established. Also, they did not find any formation of heaps. Another breakthrough is the experimental discovery of heap formation in two dimensions by Clement *et al* [11]. Using monodisperse particles, they found that (i) the static friction coefficient between the particles must be relatively large in order to induce convection and heaps, and (ii) the heap is formed as particles are being pushed upward by the sidewalls (the wall induces convection) along the surface, while there is no significant motion in the bulk. The lack of motion in the bulk is probably the consequence of hexagonal packing due to monodispersity, and not an essential part of the heap formation.

The very reason why granular particles can form a stable pile is static friction. More precisely, the contact between particles must be able to withstand a finite amount of shear

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force in order to maintain a pile. We implement static friction in MD simulations of granular material using the scheme of Cundall and Strack [12]. In this scheme, one has to apply a *finite* force in order to break a contact between particles. Using the implementations, we study heap formations in two dimensions. First, we present heap formations due to shear ('the shear-induced heaping'), which are intimately connected to 'the vibration-induced heaping'. We study the situation that sidewalls are moving vertically in opposite directions with constant velocity, thereby creating asymmetrical shear in the cell. Here, the bottom plate is not moving. We find the formation of convection *and heaps*. In these simulations, the walls are dragging nearby particles, which causes a net flux of particles. This flux is inducing convection in the cell, and the convection builds a heap, which is stable due to the presence of static friction. We also study the parameter dependence of the formation, and find that two static friction coefficients, one between the wall and a particle and the other between particles, are the most important. We next study the case that *both* walls are moving down with constant velocity, which causes symmetric shear. We also find a convection cell and heaping, whose formations are essentially the same as the asymmetric case. Next, we study the case of the vibration-induced heaping. We vibrate the sidewalls and the bottom plate of the box, and find heaps and convection cells for a range of amplitude and frequency. In particular, the heaps are formed *only* when the acceleration of the bottom plate is larger than that of gravity. Based on several measurements, we propose the following mechanism for the formation. The bottom plate is moving up or down during one half of a cycle. The density of particles are found to be smaller during the downward phase, which causes the shear force by the walls to be larger in absolute magnitude during the upward phase. Over one cycle, the net shear force applied by the wall is downward, which cause net downward flux of particles near the walls. Therefore, the vibration-induced heaping can be understood in terms of the simpler problem of the shear-induced heaping.

The force between two particles i and j, in contact with each other, is the following. Let the coordinate of the centre of particle $i(j)$ be $\boldsymbol{R}_i(\boldsymbol{R}_j)$, and $\boldsymbol{r} = \boldsymbol{R}_i - \boldsymbol{R}_j$. In two dimensions, we use a new coordinate system defined by the two vectors $\hat{n}$ (normal) and $\hat{s}$ (shear). Here, $\hat{n} = \boldsymbol{r}/|\boldsymbol{r}|$, and $\hat{s}$ is defined as rotating $\hat{n}$ clockwise by $\pi/2$. The normal component $F^{\mathrm{n}}_{j\to i}$ of the force acting on particle i by j is

$$F^{\mathrm{n}}_{j\to i} = k_{\mathrm{n}}(a_i + a_j - |\boldsymbol{r}|)^{3/2} - \gamma_{\mathrm{n}} m_{\mathrm{e}}(\boldsymbol{v}\cdot\boldsymbol{n}) \tag{1a}$$

where $a_i(a_j)$ is the radius of particle $i(j)$, and $\boldsymbol{v} = \mathrm{d}\boldsymbol{r}/\mathrm{d}t$. The first term is the Hertzian elastic force, where k_{n} is the elastic constant of the material, the constant γ_{n} of the second term is the friction coefficient of a velocity-dependent damping term, and m_{e} is the effective mass, $m_i m_j/(m_i + m_j)$. The shear component $F^{\mathrm{s}}_{j\to i}$ is given by

$$F^{\mathrm{s}}_{j\to i} = -\gamma_{\mathrm{s}} m_{\mathrm{e}}(\boldsymbol{v}\cdot\boldsymbol{s}) - \mathrm{sign}(\delta s)\min(k_{\mathrm{s}}|\delta s|, \mu|F^{\mathrm{n}}_{j\to i}|) \tag{1b}$$

where the first term is a velocity-dependent damping term similar to that of (1a). The second term is to simulate static friction, which requires a *finite* amount of force ($\mu F^{\mathrm{n}}_{j\to i}$) to break a contact [12]. Here, μ is the friction coefficient, δs the *total* shear displacement during a contact, and k_s the elastic constant of a virtual spring. There are several studies on granular systems using the above interactions [13]. However, only a few of them [12, 14, 15] include static friction. A particle can also interact with a wall. The force on particle i, in contact with a wall, is given by (1) with $a_j = \infty$ and $m_{\mathrm{e}} = m_i$. A wall is assumed to be rigid, i.e. it is not affected by collisions with particles. Also, the system is under a gravitational field $\boldsymbol{g}$. We do not include the rotation of the particles in the present simulation. A detailed explanation of the interaction is given elsewhere [15].

We first consider the situation that systems of granular particles are under constant vertical shear. Consider a box of width W and height H. We insert particles at randomly chosen positions inside the box, and calculate the trajectories of the particles by a fifth-order predictor–corrector method. The particles fall by gravity, lose their energy through collisions, and fill the box without any significant motion. The parameters we use for the interaction between the particles are $k_n = 1.0 \times 10^6$, $k_s = 1.0 \times 10^4$, $\gamma_n = 1.0 \times 10^3$, $\gamma_s = 0$ and $\mu_{pp} = 0.2$. For the interaction between the particle and the wall, we use $k_n = 2.0 \times 10^6$, $k_s = 1.0 \times 10^4$, $\gamma_n = 5.0 \times 10^2$, $\gamma_s = 0$. The friction coefficient at the sidewall and bottom plate are $\mu_{pw} = 5.0$ and 0.2, respectively. The time-step is chosen to be 5×10^{-5}, and gravity g is 980. In this letter, CGS units are implied. In order to avoid the hexagonal packing formed by particles of the same size, we choose the radius from a Gaussian distribution with average 0.1 and width 0.02. The density of the particles is chosen to be 0.5. We then apply a vertical shear by pulling the right (left) wall with constant velocity $v_s = 0.2$ (-0.2). In figure 1(a), we show the system after 80 000 iterations of the vertical shear. The slope of the surface of the pile increases, and fluctuates around a non-zero value. The mechanism to generate the heap is rather simple. Since one pulls the sidewalls with constant velocity, the walls exert shear forces to nearby particles. If the force at the wall is sufficiently high, it will induce flow of particles in the vertical direction. The upward (downward) flow of particles near the right (left) wall, combined with static friction, results in the formation of the heaps.

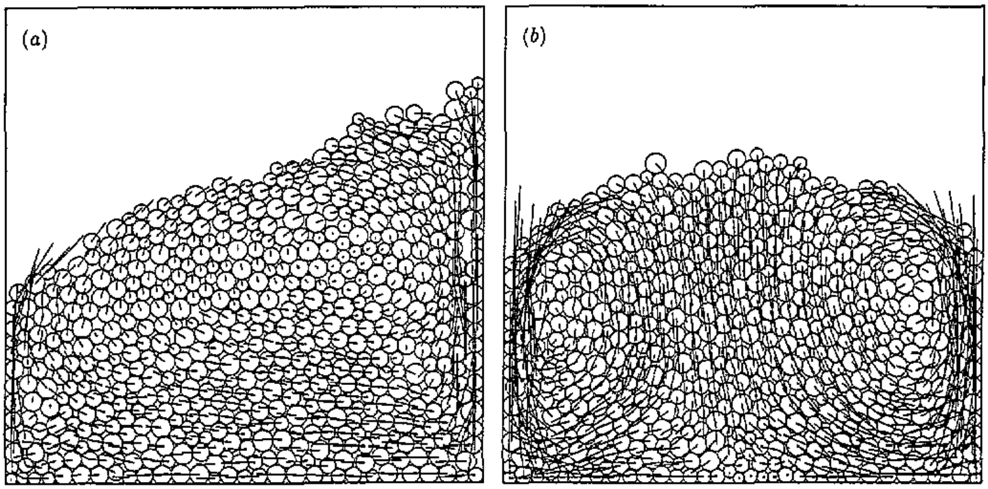

Figure 1. Shear-induced heap formations. (a) Configuration after 80 000 iterations of asymmetric shear where the right (left) wall is moving up (down) with constant velocity $v_s = 0.2$. The total displacement of particle i over the period are shown by lines joining the present r_i (with circle) to the initial r_i. (b) Configuration after 50 000 iterations of symmetric shear, where both walls are moving down with constant velocity $v_s = -1.0$.

We study the effect of parameters on the formation of the heaps. There are quite a few parameters in the system. However, most parameters, while their values are chosen within reasonable ranges, do not affect the behaviour of the system. The key parameters are the two friction coefficients μ_{pw} and μ_{pp}, and the shear velocity of the sidewalls v_s. First, we study the effect of μ_{pw}. We fix $\mu_{pp} = 0.2$, $v_s = 0.2$, and the friction coefficient of the bottom plate to be zero. For small μ_{pw} (0.5 or 1.0), the particles do not move significantly during the whole simulations, which results in a zero angle. In order to have convective motion and heaping, $\mu_{\rm pw}$ should be larger than certain threshold $\mu_{\rm pw}^{\rm c}$. The existence of a finite threshold $\mu_{\rm pw}^{\rm c}$ can be understood as follows. In order to lift particles near the right wall, the shear force by the right wall should be larger than the sum of the gravitational force and the friction between particles. Since the sum is finite, one needs finite $\mu_{\rm pw}$ in order to maintain the convection. It is still an open question whether the transition is the first or the second order, i.e. whether there exists a sudden jump of $\langle\theta\rangle$.

We now fix $\mu_{\rm pw} = 5.0$, $v_{\rm s} = 1.0$, and study the effect of $\mu_{\rm pp}$. We calculate $\langle\theta\rangle$ for several values of $\mu_{\rm pp}$, where the averages are taken over approximately 1000 points. Here, $W = 3$ and $n = 150$. The angle $\langle\theta\rangle$ becomes larger for larger values of $\mu_{\rm pp}$, which may result from the fact that the angle of repose is an increasing function of $\mu_{\rm pp}$ [15]. We then study the effect of $v_{\rm s}$ by fixing $\mu_{\rm pw} = 5.0$, $\mu_{\rm pp} = 0.2$, and change $v_{\rm s}$. We measure $\langle\theta\rangle$ for several values of $v_{\rm s}$ between 0.1 and 10.0 with $W = 3$, $n = 150$. The measured angle is quite insensitive to $v_{\rm s}$. For example, the angle is 25.8 for $v_{\rm s} = 0.1$ and 23.6 for $v_{\rm s} = 10.0$. When $v_{\rm s}$ is increased, the pile tries to increase the slope due to larger current of particles. On the other hand, increased motion of particles decreases the stabilizing effect of static friction. These two effects seem to cancel each other resulting in the insensitive dependence.

So far, we have studied the formation of heaps by an asymmetric shear, i.e. the sidewalls are moving in the *opposite* direction. We now consider the case of a symmetric shear, where both sidewalls are moving in the *same* direction. In figure 1(*b*), we show the system after 50000 iterations. Here, we use $\mu_{\rm pw} = 5.0$, $\mu_{\rm pp} = 0.2$, and both walls are moving down with constant velocity $v_{\rm s} = -1.0$. The mechanism of generating the symmetric heap shown in the figure is essentially the same as that of the asymmetric heap. The shear force induces downward flow of particles near the sidewalls. The flow merges together around the centre of the cell, and rises to the top of the pile.

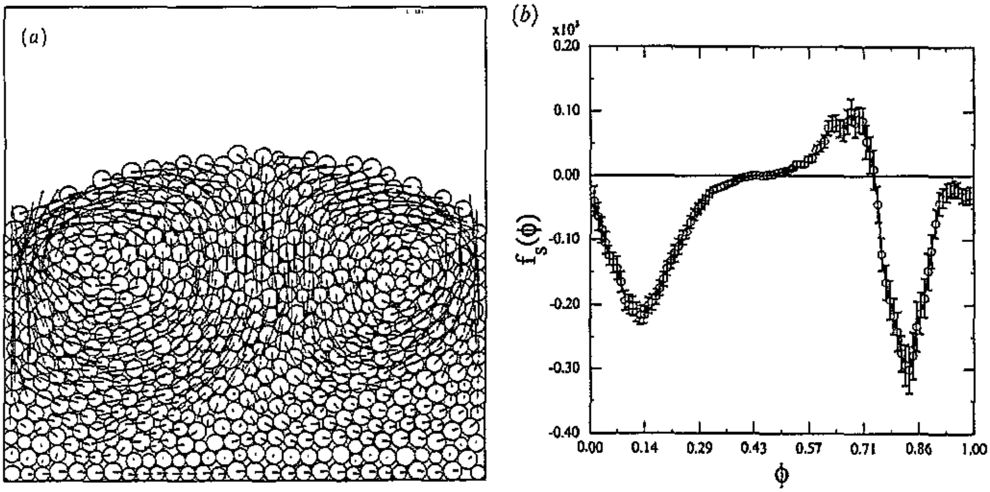

Figure 2. (*a*) Vibration-induced heap formation. Configuration after 16 cycles of vibration with vibrating bottom plate and fixed sidewalls. Displacements of particles over 15 cycles are also shown. (*b*) We show the shear force $f_s(\phi)$ for the different phases ϕ.

We want to argue that the above 'shear induced heaping' is related to the 'vibration induced heaping'. In fact, the above shear geometries are chosen to demonstrate more clearly their similarity. We now study the vibration induced heaping, and discuss its relation to the shear-induced case. We vibrate the sidewalls of a box as well as the bottom plate with amplitude A and frequency f. In figure 2(a), we show the system after 40 cycles as well as the displacements of the particles over 10 cycles. For this simulation, we take $W = 6$, $n = 600$, $A = 0.250$ and $f = 10$ Hz. The parameters for the interaction between the particles and the sidewall are $\mu = 5.0$, $\gamma_n = 1.0 \times 10^3$. For the interaction between the particles, we use $\mu = 0.2$. All the other parameters are kept to be the same as before. In the figure, one can see a heap and associated convection. We measure the angle of the heap for a few runs using the above parameters. The angle increases for about the first ten periods of the vibration, then just fluctuates with mean 10.2 and standard deviation 2.1. Here, the averages are taken over a total of 230 periods.

We now discuss the mechanism for the formation of the heap. The average number of particles $c(\phi)$ in contact with one particle for various phases ϕ during one cycle is measured. The phase ϕ is measured in the unit of 2π. The numbers $c(\phi)$ are smaller during the downward phase ($0.25 < \phi < 0.75$) than the upward phase. One of the consequences of this 'up/down symmetry breaking' is the shear forces of the sidewalls are also asymmetric. In figure 2(b), we show the total shear force $f_s(\phi)$, which the right wall applies to the particles, for several values of ϕ. The sign of f_s is roughly opposite to that of the velocity of the bottom. The absolute magnitude of f_s is larger for the upward phase, and because the particles are more densely packed, the wall can exert a larger force. Since the shear force is essentially a drag force for the particles, we expect particles move faster vertically during the downward phase, where the shear force is smaller. Therefore, there is net downward flux of particles near the sidewalls, which results in a convective motion and heaping. In summary, the convection and heaping is due to the net current along the sidewalls, which is caused by the net downward shear, which again is a result of 'up/down symmetry breaking' of the particle density.

We now study the effects of various parameters on the formation of heaps under the vibration. The formation is greatly affected by the two main ingredients, the net shear force which drives the convection, and the static friction which stabilize heaps. First, we change the mean height of the pile to 10, 20 and 30 particle diameters (layers). We also change the amplitude A, but the other parameters are kept to be the same as above. For the systems of 20 and 30 layers, we find heaps for $A = 0.250$ ($\Gamma = 1.01$) and 0.275 ($\Gamma - 1.11$), but we do not find a heap for $A = 0.200$ ($\Gamma - 0.80$) and 0.300 ($\Gamma - 1.21$). On the other hand, no heap is found for the system of 10 layers. Here Γ is the ratio of the acceleration of the bottom plate to that of gravity. This dependence on the height can be understood as follows. The static friction, which stabilize the heap, acts *only* between particles in contact. Since the distances between the particles become larger as the number of layers is decreased [16], the static friction becomes less effective, and the heaps become less stable. This can explain why heaps are found only with large number of layers.

We now discuss the effect of the amplitude A. If A is so small that Γ becomes less than 1, the acceleration of the box is smaller than that of gravity. The particles cannot lose contact, and there are no net displacement of the particles relative to the sidewalls. Therefore, there is no net shear force, and as a result no convection. In contrast, we find *heap and convection* even for $\Gamma < 1$, when we fixed the sidewalls and vibrate only the bottom. In this case, the particles *do* move relative to the sidewalls even for $\Gamma < 1$, and therefore the net shear force is produced by the sidewalls. As A becomes large, the distances between the particles also become large, and heaps become less stable. Therefore, if Γ becomes too large, we expect convection without associated heap, which is exactly what we observe in the simulations. It is also consistent with the experimental observation that there are ranges of A ('window') for the formation of heaps [17]. However, the width of the window found above ($\Delta\Gamma \sim 0.1$) is much smaller than that found in experiments ($\Delta\Gamma \sim 4$) [17]. This discrepancy can be due to the fact that $\Delta\Gamma$ depends on the interaction parameters of the system. Indeed, we find larger $\Delta\Gamma$ for larger values of γ_n (varied between γ_n to 2×10^3). We also study the effect of the friction coefficient μ. We first fix μ_{pw} to be 5.0, and change μ_{pp}. As we increase μ_{pp} from 0.2, the steady-state angle of the heap starts to increase, but heap (and convection) disappears for $\mu_{pp} = 1.0$. The friction between the particles increase as μ_{pp} is increased, and therefore the net shear force needed to produce the convection should also increase for large μ_{pp}. This argument is checked by the fact that there is convection and heap for $\mu_{pp} = 1.0$, when we increase $\mu_{pw} = 10.0$, by which the shear force is increased.

It has been observed previously that walls are reasonable for the convection and/or the formation of heaps, and there have been conflicting arguments on the way how the walls *induce* the convection [9–11]. We presented here an argument based on measuring properties of the system. Our argument is similar to that of Gallas *et al* [10] in the sense that both are based on the shear force that the walls are exerting on the particles.

In conclusion, we find heap formations in two types of systems—one with constant vertical shear, the other with a vibrating bottom and sidewalls. We also presented qualitative mechanism for the formations of heaps in these systems. Heaps in both systems are caused by a net downward shear. In both systems, there are many interesting quantities to measure. In the vibration-induced heaping, it would be nice to check for the existence of a net shear by measuring the shear stress of the walls. It would be important to study the parameter dependence of the angle of the heaps formed by the vibration. In the shear-induced case, further understanding of parameter dependences of $\langle\theta\rangle$ (especially μ_{pw}) is necessary experimentally as well as theoretically. Unfortunately, heap formation in three dimensions cannot be explained by this mechanism, since it is known that heaps can be formed without a boundary in 3D. The mechanism for 3D heap formation still remains to be understood.

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