Heap Formation in Granular Media

Jysoo Lee

HLRZ-KFA Jülich, Postfach 1913, W-5170 Jülich, Germany

Abstract

Using molecular dynamics (MD) simulations, we find the formation of heaps in a system of granular particles contained in a box with oscillating bottom and fixed 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.

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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 cell under vibration.\textsuperscript{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.\textsuperscript{5} However, even with many recent studies on the subject,\textsuperscript{6−11} the exact mechanism for the heap formation is not established.

Recently, two experimental groups, Evesque \textit{et al}\textsuperscript{6} and Laroche \textit{et al},\textsuperscript{7} studied behaviors 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 \textit{et al} find convection but no heap.\textsuperscript{8} When viewed from above, these boxes are essentially squares, making the system fundamentally 3-dimensional. On the other hand, there are some studies in 2 dimension (i.e. a line when viewed from above) with fruitful results. Using molecular dynamics (MD) simulations of granular particles, Taguchi\textsuperscript{9} and Gallas \textit{et al}\textsuperscript{10} found convection cells under vibration in 2 dimension. Furthermore, they established the fact that the sidewalls are \textit{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 heap. Another breakthrough is the experimental discovery of heap formation in 2 dimension by Clement \textit{et al}.\textsuperscript{11} Using monodisperse particles, they found that (1) the static friction coefficient must be relatively large in order to induce convection and heap, and (2) 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
force in order to maintain a pile. We implement static friction in MD simulations of granular material using the scheme of Cundall and Strack. 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 2 dimension. 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 heap. 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 the 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. Finally, we study the case of vibration induced heaping. We first fix the sidewalls and vibrate the bottom plate. We find heap formation and convection for a range of amplitude and frequency. 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 cause 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 situation is very similar to the case of the symmetric shear. We also study the case of vibrating the sidewalls as well as the bottom plate, and find convection but no heap. We discuss possible explanation.

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

$$F^n_{j\rightarrow i} = k_n(a_i + a_j - |\vec{r}|)^{3/2} - \gamma_n m_e (\vec{v} \cdot \hat{n}),$$  \hspace{1cm} (1a)$$

where $a_i$ ($a_j$) is the radius of particle $i$ ($j$), and $\vec{v} = d\vec{r}/dt$. The first term is the Hertzian elastic force, where $k_n$ is the elastic constant of the material. And, the constant $\gamma_n$ of the second term is the friction coefficient of a velocity dependent damping term, $m_e$ is the effective mass, $m_i m_j/(m_i + m_j)$. The shear component $F^s_{j\rightarrow i}$ is given by

$$F^s_{j\rightarrow i} = -\gamma_s m_e (\vec{v} \cdot \hat{s}) - \text{sign}(\delta s) \min(k_s |\delta s|, \mu |F^n_{j\rightarrow i}|),$$  \hspace{1cm} (1b)$$

where the first term is a velocity dependent damping term similar to that of Eq. (1a). The second term is to simulate static friction, which requires a finite amount of force ($\mu F^n_{j\rightarrow i}$) to break a contact. Here, $\mu$ is the friction coefficient, $\delta s$ 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. However, only a few of them include static friction. A particle can also interact with a wall. The force on particle $i$, in contact with a wall, is given by Eqs. (1) with $a_j = \infty$ and $m_e = m_i$. 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 $\vec{g}$. We do not include the rotation of the particles in present simulation. A detailed explanation of the interaction is given elsewhere.

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 $5 \times 10^{-5}$, 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. Later, we also study the system of monodisperse particles. We then apply a vertical shear by pulling the right (left) wall with constant velocity $v_s = 0.2 (-0.2)$. In Fig. 1(a), we show the system after 80000 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.

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 behavior of the system. The key parameters are the two friction coefficients $\mu_{pw}$ and $\mu_{pp}$, and the shear velocity of the sidewalls $v_s$. First, we study the effect of $\mu_{pw}$. We fix $\mu_{pp} = 0.2$, $v_s = 0.2$, and the friction coefficient of the bottom plate to be zero. In Fig. 1(b), we show the average angle of the pile $\langle \theta \rangle$ for different values of $\mu_{pw}$ with $W = 3$ and the number of particles $n = 150$. Here, averages are taken over time (excluding the transient) and several different runs, where each angle is averaged over approximately 5000 points. For small $\mu_{pw}$ (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, $\mu_{pw}$ should be larger than certain threshold $\mu_{pw}^c$. The existence of a finite threshold $\mu_{pw}^c$ 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 $\mu_{pw}$ 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 $\mu_{pw} = 0.2$, $v_s = 1.0$, and study the effect of $\mu_{pp}$. We calculate $\langle \theta \rangle$ for several values of $\mu_{pp}$, 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 $\mu_{pp}$, which may results from the fact that the angle of repose is an increasing function of $\mu_{pp}$. We then study the effect of $v_s$ by fixing $\mu_{pw} = 5.0$, $\mu_{pp} = 0.2$, and change $v_s$. We measure $\langle \theta \rangle$ for several values of $v_s$ between 0.1 and 10.0 with $W = 3$, $n = 150$. The measured angle is quite insensitive to $v_s$. For example, the angle is 25.8 for $v_s = 0.1$ and 23.6 for $v_s = 10.0$. When $v_s$ 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 to the insensitive dependence. Finally, we study the same system using monodisperse particles. The system just before we apply the shear is a hexagonal packing of particles with few defects. When the shear of $v_s = 0.2$ is applied, the hexagonal packing becomes unstable, and the system starts to form a square packing. When the formation of the square packing is completed, the particles near the wall can withstand the applied shear with no motion. The square packing, which is stable for small values of shear, becomes unstable as $v_s$ is increased.

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 Fig. 1(c), we show the system after 50000 iterations. Here, we use $\mu_{pw} = 5.0$, $\mu_{pp} = 0.2$, and both walls are moving down with constant velocity $v_s = -1.0$. 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 center of the cell, and rises to the top of the pile.

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 with the shear induced case. We first fix both sidewalls of a box and vibrate the bottom plate with amplitude $A$ and frequency $f$. In Fig. 2, we show the system after 16 cycles as well as the displacements of the particles over 15 cycles. For this simulation, we take $W = 10$, $n = 800$, $A = 0.190$ and $f = 20 \text{Hz}$. The parameters of the interaction of the particles and the sidewall are $\mu = 3.0$, $k_s = 1.0 \times 10^6$. For the interaction between the particles, we use $\mu = 0.5$ and $k_s = 5.0 \times 10^4$. All the other parameters are kept the same as before. In the figure, one can clearly see a heap and associated convection.

We now discuss the mechanism for the formation of the heap. In Fig. 2, we show the average number of particles $c(\phi)$ in contact with one particle for various phases $\phi$ during one cycle. Here, $\phi$ is in the unit of $2\pi$, and the averages are taken over 20 cycles. 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 Fig. 2, we show the total shear force $f_s(\phi)$, which the right wall applies to the particles, for several values of $\phi$. 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 consider a similar case when we vibrate the sidewalls as well as the bottom plate. We find that the above mechanism still holds—there is net downward shear and flux of particles near the wall, and convection cells. However, we do not find a heap. To understand this, we note that the vibration, which is the source of convection and heaping, also tends to make an existing heap unstable. The shear force, which is the driving force of the convection, is proportional to the relative shear displacement between the walls and particles due to the present implementation scheme of static friction. With fixed walls, we can obtain rather large net shear force for small $A$, even when the acceleration of the bottom is smaller than $g$. With moving walls, however, we need the acceleration to be at least as large as $g$ to have the relative displacement and net shear. For large $A$, the vibration induces motion of particles along the top surface, which dominates the current due to the convective motion. This destroys any existing heap. This observation does not necessarily imply that there is no heap formation with moving walls in 2-dimension. It has been known that there are some range of $A$ (“windows”) for the formation of a heap.\textsuperscript{16} The width of the window is very likely to be dependent on the parameters of the material. The window may be very narrow for the range of parameters we are studying. A similar parameter problem could also explain why no heap was found in the experiment by Zik \textit{et al.}\textsuperscript{8}. There is limitation on the range of parameters we can simulate. For example, $k_s$ is very large (ideally, infinity) for real material, and larger $k_s$ is more effective in creating convection. However, we can not simulate values of $k_s > 1.0 \times 10^6$ without significantly decreasing the time step. The situation is entirely similar with $\gamma_n$—we can not increases $\gamma_n$ beyond $1 \times 10^3$. As a result, it is possible that the heap can be found in these parts of the parameter space.

It has been observed previously that walls are responsible for the convection and/or the formation of heaps, and there have been conflicting arguments on the way how the walls
We presented here an argument based on measuring properties of the system. Our argument is similar to that of Gallas et al in the sense that both are based on the shear force that the walls are exerting on the particles. However, the two theories have different mechanisms for the generation of the net shear force.

In conclusion, we find heap formations in two types of systems—one with constant vertical shear, the other a with vibrating bottom and fixed walls. Heaps in both systems are caused by a net downward shear. Both of the systems are not studied experimentally, and 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 repose. In the shear induced case, the further understanding of a parameter dependences of \( \langle \theta \rangle \) (especially, \( \mu_{pw} \)) is necessary experimentally as well as theoretically. Unfortunately, heap formation in 3 dimension can not be explained by this mechanism, since it is known that heaps can be formed without a boundary in 3-d. The mechanism for 3-d heap formation still remains to be understood.

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Figure Captions

Fig. 1: Shear induced heap formations: (a) Configuration after 80000 iterations of asymmetric shear where the right (left) wall is moving up (down) with constant velocity $v_s = 0.2$. (b) The dependence of the angle of repose $\langle \theta \rangle$ on the friction coefficient of the wall $\mu_{pw}$. (c) Configuration after 50000 iterations of symmetric shear, where both walls are moving down with constant velocity $v_s = -1.0$.

Fig. 2: 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. In the insets, we also show the average number of contact $c(\phi)$ and the shear force $f_s(\phi)$ for the different phases $\phi$. 