Hexagonal close-packed stability in two-dimensional self-gravitation granular particles system

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Abstract. Spherical grains in equal size were initially set in nearly hexagonal close packed configuration. The particles were separated in 0.1 ± 0.05 d distance in order to generate the initial vibration to the system. We set two grains as intruders, which mass and position will be adjusted in simulation. Previously, we have conducted simulation of self-gravitation granular particle system to predict the formation of asteroid and results the hexagonal close packed configuration at the end of simulation as consequence of saturation value of contactopy. In this work, we found that the hexagonal close packed system can be destructed by certain arrangement of particles and intruders.

1. Introduction
The idea of analysing the self-gravitation granular particle system comes from the prediction of formation of asteroid that is similar to the Brazil Nut Effect (BNE) phenomenon [1]. A number of grains in different size and mass which separated in certain distance will be attracted due to gravitational force, and forming an aggregate of particle via inelastic collision [2]. The formation process is considered to be completed when the number of contactopy reaches the saturation value [3]. The densest number of contactopy for spherical grains in equal size can be achieved through two-dimensional hexagonal close packed (HCP) formation. This formation has a stable structure due to low potential energy in uniform distribution of particle mass.

In this work, we are going to analyse the stability of two-dimensional HCP structure by placing two particles with larger mass, which is then referred to as intruder, in various position. We set the grains in nearly HCP formation to attract the grains to form an ideal HCP, yet it does not rule out the possibility for the grains to form different configuration other than HCP.

2. Model
In this research, the two-dimensional particle system with particle diameter d was set in nearly HCP formation. We remove the particle at the centre of system in order to allow the particles form different structure other than hexagonal close packed in simulation.
Particle number \( i \) start at 0 and layer number \( j \) start at 1. The number of particle \( N \) is depend on the number of layer, following the equation below:

\[
N = 6 \sum_{n=1}^{J} n
\]  

(1)

where \( J \) is number of layer. First layer of hexagon would have 6 particles, thus first 2 layers of hexagon will be consist of \( 6(1+2) \) particles. The number of particles in some layers is described in figure 2.

The angular position for particle-\( i \) and \( i+1 \) is separated by \( \Delta \theta \), which is depend on the layer number \( j \). The angular positions were arranged by the following equations:

\[
\theta_{i+1} = \theta_i + \Delta \theta
\]

(2)

\[
\Delta \theta = \frac{2\pi}{6j}
\]

(3)

By using equation (2 – 3), the visualisation of angle difference is shown by figure 3, where the angle difference based on equation (3) are fit to the particle position in the first and second layer. While in the third layer, the calculated angle could not satisfy the particle position in HCP configuration. Thus we call this formation as a nearly hexagonal close packed system.
Figure 3. Angle difference between particles for (a-b) first layer, (c) second layer, and (d) third layer.

The position of particles was divided into 2 groups: the particles at the corners and at the sides. Particles at the corners, which have angular position $\theta$ of $i\pi/6$, were arranged by the equation below

$$x_i = jd \cos \theta_i$$

$$y_i = jd \sin \theta_i$$

while at the sides, the particles with $\theta_i$ other than $i\pi/6$ were positioned by

$$x_i = jd - \frac{(j-1)d}{2j} \cos \theta_i$$

$$y_i = jd - \frac{(j-1)d}{2j} \sin \theta_i$$

In simulation program, the value of $j$ will be automatically increased by $1 \times j$ when the angular position met $2\pi$ according to equation (2).

2.1. Interaction Forces

Interaction between two particles with considerable mass $m_1$ and $m_2$ separated by $r_{ij}$ is described by gravitational force

$$\vec{G}_{ij} = g \frac{m_1 m_2}{r_{ij}^2} \hat{r}_{ij}$$

where $g$ is gravitational constant with value about $6.674 \times 10^{-11}$m$^3$kg$^{-1}$s$^{-2}$. In simulation, we used higher value of gravitational constant in order to accelerate the effect of the force to the particle movement. Repulsion force that generated from the collision between particles [4] is

$$\vec{N}_{ij} = \left( k_N \xi_{ij} - \gamma_N \frac{d\xi_{ij}}{dt} \right) \hat{r}_{ij}$$

The particle motion can be derived from equation (7) and (8) using Euler method [4].
3. Simulation

This event driven simulation is built by JavaScript and HTML as the interface [5].

Figure 4. Initial condition of simulation with 58 bed particles and 2 intruders, numbered 36 and 48, separated by 180° angle difference.

Bed particles were marked with blue line and intruders marked with red line. We varied the initial distance between intruders by changing the angular position of intruder other than numbered 36. Ratio of intruders mass and bed particle $M:m$ was varied from 1:1 to 10:1 with increment of $m$ in each position. In initial condition, the particles are separated by $0.1 d \pm 0.05 d$ to generate initial vibration between particles.

Figure 5. Variation of intruder's initial position with (a) ~15°, (b) ~30°, (c) ~45°, (d) 60°, (e) ~75°, (f) 90°, (g) ~105°, (h) 120°, (i) ~135°, (j) ~150°, (k) ~165°, and (l) 180° angle difference.
In this simulation, we assume that the intruder position on the upper line (number 48 to 59) will have the same behaviour with the lower line (37 to 47). For example, if we set the condition of particle number 36 and 50 as the intruders, it will obtain the same result as particle 36 and 46. Thus we consider to take the upper line and assume there was a horizontal symmetry with the lower line.

The interaction between intruders will be greater than other particles due to the mass. The presence of void at the centre would allow the intruder to push the bed particles around, when the force between intruders is considerable. This condition can be analysed quantitatively by measuring the distance between intruders, from initial to final condition.

4. Result and Discussion
The simulation runs until \( t = 1.5 \) s, when the vibration of particles has decreased. When the forces are working in the system, the particles tend to move to the centre of the system. Generally, there are three groups of final condition, (i) ideal two-dimensional HCP, (ii) broken two-dimensional HCP with small void inside, and (iii) broken two-dimensional HCP with no void inside. These three conditions are described in figure 6.

![Figure 6](image1)

Figure 6. Three groups of final condition at 180° angle difference with various intruder mass (a) ideal two-dimensional HCP when \( M = 2 \) m, (ii) broken two-dimensional HCP with small void inside when \( M = 6 \) m, and (iii) broken two-dimensional HCP with no void inside when \( M = 10 \) m.

The configuration of these three final conditions is depend on the mass and initial position of intruders. Figure 6b shows a broken HCP with small void inside yet stable to resist the force by intruders. While \( M:m = 10:1 \), which was shown in figure 6c, resulted a broken HCP with no void inside. The 180° angle difference leads the vertical symmetry on the final condition.

![Figure 7](image2)

Figure 7. Transformation of particles for \( M = 2m \) with \(-165°\) angle difference when (a) \( t = 0.2 \) s, (b) \( t = 0.4 \) s, (c) \( t = 0.8 \) s, and (d) \( t = 1 \) s resulting an ideal two-dimensional HCP formation.

System with \( M:m = 2:1 \) and \(-165°\) angle difference resulted an ideal two-dimensional HCP formation even though the initial condition was not a perfect HCP. At the same position, with \( M:m = 10:1 \) resulted a broken hexagonal along with the loss of void. The intruders have a strong attraction force and push the bed particles around the void.
Figure 8. Transformation of particles for $M = 10$ $m$ with $\sim 165^\circ$ angle difference when (a) $t = 0.2$ $s$, (b) $t = 0.4$ $s$, (c) $t = 0.8$ $s$, and (d) $t = 1$ $s$ resulting a broken two-dimensional HCP formation with no void at the centre of system.

Even though the broken 2-d HCP in figure 8d and figure 6c has no void inside, they had different structure of broken HCP. This condition is caused by the initial position, where the intruders in figure 8 were not in the symmetrical position.

Figure 9. Transformation of particles for $M = 9$ $m$ with $\sim 30^\circ$ angle difference when (a) $t = 0.2$ $s$, (b) $t = 0.4$ $s$, (c) $t = 0.6$ $s$, and (d) $t = 1$ $s$, HCP formation was broken by the interaction between intruders.

By arranging the intruders in small angle difference, but not adjacent, the mass of the system will be localized according to the position of intruders. We took $\sim 30^\circ$ as the example for this condition, which can be seen in figure 9. As shown in figure 9a, the particles on the left side, where the intruders are located, start to contact at $t = 0.2$ $s$, whereas the particles on the right side still separated by small distance. The forces between intruders can shift the position of bed particles in between, which was particle number 59. This movement affected the other particles around intruder, such as number 27 and 37. This condition can also be obtained at $\sim 45^\circ$ angle difference, where the intruders were particle number 36 and 57.

Generally, the final position was grouped into three conditions, short, medium, and long distance change, except the positions below $\sim 30^\circ$ which have 1 and 2 final conditions. For $\sim 15^\circ$ angle difference, the intruders are adjacent at the initial position, thus the intruders will only have one final condition for all value of mass.
Figure 10. The changes of distance between intruders, grouped by initial position (a) ~15°, (b) ~30°, (c) ~45°, (d) 60°, (e) ~75°, (f) 90°, (g) ~105°, (h) 120°, (i) ~135°, (j) ~150°, (k) ~165°, and (l) 180° angle difference. (--- = m, --- = 2 m, --- = 3 m, --- = 4 m, --- = 5 m, --- = 6 m, --- = 7 m, --- = 8 m, --- = 9 m, --- = 10 m).

5. Conclusion
The built program can be used to simulate nearly-HCP formation with various number of particles. When two intruders with mass 7 to 10 times larger than the bed particles placed in the HCP formation, they tend to break the formation by reducing the void inside the system. Whereas the angle difference between intruders was ~30° and ~45°, it will allow the intruders to contact by shifting the bed particles in between. Further research, this concept could be applicable for three-dimensional system.
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Reference
[1] G V Punyakoti, Brazil nuts help unlock the asteroid’s boulder mystery, Current Science 107 (2014), p. 945-946.
[2] V Perera, A P Jackson, E Asphaug, R L Ballouz, The spherical brazil nut effect and its significance to asteroids, Icarus 278 (2016), pp. 194-203.
[3] S Viridi and B Dermawan, Tumbukan tak-elastik partikel sebagai model terbentuknya asteroid, Spektra: Jurnal Fisika dan Aplikasinya 2 (2017), pp. 53-60.
[4] S Viridi and R Kurniadi, Komputasi Fisika 3: Simulasi dan Visualisasi Fisika dengan JavaScript, Departemen Fisika, FMIPA, Institut Teknologi Bandung (2017), pp. 289 – 294 doi: 10.13140/RG.2.2.35065.67680.
[5] D C Richardson, K J Walsh, N Murdoch, P Michel, Numerical simulations of granular dynamics: I. Hard-sphere discrete element method and tests, Icarus 212 (2011), p. 427-437.