Cluster compaction of two-dimension spherical particles binary mixture as model of forming process of an asteroid

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Abstract. Several two-dimension spherical particles are under influence of gravitational forces of each other and as they are colliding repulsion forces in form of linear spring-dashpot prevent them from collapsed into a single point. Gravitational constant larger than $G$ is used for better and faster stabilization in forming cluster of the particles, accompanied with values of $k = 10^4$ N/m and $\gamma = 0.5$ N·s/m As initial conditions the particles are placed randomly with separation distances among each other. Molecular dynamics method implementing Euler algorithm is used to simulate the developing of particles cluster, which is intending to mimic the process of an asteroid forming. Time step of $\Delta t = 10^{-2}$ s is chosen and results are reported every some period from 1 s to 1000 s, where after each period all particles velocity are forced to be zero. It is observed that not only physical parameters influencing the compaction of the asteroid but also simulation parameters.

1. Introduction

Asteroids are small bodies in our solar system whose surfaces have various features. There are high and low topography, large and small craters, boulders, small rocky materials, and regolith. From spectroscopy observations, taxonomy of asteroids provides several major surface types, i.e. carbonaceous, silicate and metallic. Solar wind and other space weathering process are believed to alter the spectral color of many types of asteroids. Asteroid rotates on its axis during its revolution orbiting the Sun. Some properties of internal structure of asteroid can be derived from its lightcurve. There are a barrier of rotation period of 2.2 hours for sizes of 1 km or larger, and remarkably, for sizes below 100 m the rotation periods can be 5 minutes [1]. This constrains its bulk density and level of (macro)porosity. Two examples of asteroids having distinct internal structure are 253 Mathilde (bulk density 1.3 g/cm³, porosity 50%) and 216 Kleopatra (bulk density 6 g/cm³, equilibrium figure of iron/metal) [1]. Results from some asteroid missions, e.g. to 433 Eros and 25143 Itokawa, have shown that asteroids are gravitational aggregate bodies (rubble-pile), not monolithic structure. However, for much smaller size of asteroids, whose rotation periods are very fast, it is believed that they are indeed monolithic bodies. There are many unexplained features and distribution of materials on asteroid surface. Smooth regolith and large rocky materials can be found side by side. Impact can shake seismically the asteroid body, so that surface and sub-surface materials can be changed and mixed [2].
Recent exploration of Hayabusa mission to Itokawa asteroid has successfully brought high resolution images showing how boulders, gravels, and sands distributed on its surface, where they have some preferred orientation at some places but not in other places [3]. Occurrences of larger particles, e.g. boulders, above smaller particles, e.g. gravel or sand, are addressed to the well-known phenomenon in granular world, i.e. the Brazil-nut effect (BNE) [4]. Simulation in 2-d, which is conducted under influenced only of gravitation of granular particles in the system, shows that there is a ring of larger particles formed near the edge of the granular aggregate [5]. Even further, collision of two such aggregates for much smaller particles has also been reported [6]. On earth surface, where gravitation is always toward center of the planet, decrease of porosity and increase of contactopy is observed during the process of BNE [7], which is interesting to observe it in the system under influence of gravitation of its own particles.

2. Simulation

Particles which later forming an asteroid are simplified into 2-d spherical particles, each with the same density $\rho$, while for each particle $i$ the diameter $D_i$ and mass $m_i$ may be varied. Only two types of forces between particles are considered in this work. The former is gravitation force while the later is normal force. In order to get particles motion variables such as velocity and position, molecular dynamics (MD) method is used, which implementing Euler algorithm.

2.1. Forces formulation

Two types of force are considered, gravitation force $F_G$ and and normal force $F_N$ [8]

$$
\vec{F}_G = -k_G \frac{m_i m_j}{r_{ij}^2} \hat{r}_{ij} \tag{1}
$$

$$
\vec{F}_N = \left( k_N \hat{r}_{ij} - \gamma_N \frac{d\hat{r}_{ij}}{dt} \right) \hat{r}_{ij}. \tag{2}
$$

![Figure 1. Total force $F_{\text{total}}$ for $D_i + D_j = 2$, $k_N = 10^4$, and $G = 10^{-7}$, where $F_N$ dominates for small range of $r_{ij}$ and $F_G$ dominates for large range of $r_{ij}$.](image)

It can be seen in figure 1 that $F_N$ dominates in short range while $F_G$ in long range of distance between particles $r_{ij}$. Notice that values of $F_N$ and $F_G$ have different scale in order of magnitude. The distance about 0.999297 (can not be seen in figure 1) is equilibrium distance, where $F_N = F_G$.

2.2. Molecular dynamics (MD) method

The MD method has two steps: i. calculation of acceleration of all particle, and ii. calculation new velocity and new position of all particle. The first step is conducted using Newton second law of motion

$$
\ddot{a}_j(t) = \frac{1}{m_j} \sum_{j \neq i} \left[ \vec{F}_G^{ij}(t) + \vec{F}_N^{ij}(t) \right] \tag{3}
$$

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and the second step can be performed using various numerical algorithm, but improved Euler algorithm is chosen in this work due to its simplicity

\[ (\vec{v}, \vec{r})(t + \Delta t) = (\vec{v}, \vec{r})(t) + (\vec{a}, \vec{v})(t) \Delta t. \]  

Equations (4) are executed repeatedly until termination condition is reached.

2.3. Number of contact points

From contact energy \( U \) [9] formulation of number of contact points can be derived

\[ N_c(t) = \frac{\partial U_c(t)}{\partial \gamma} \approx \sum_{i,j \neq i} \text{sign} \left[ \varepsilon_{ij}(t) \right]. \]  

2.4. Microstates and macrostates

For \( L \geq 2 \) the macrostates are defined slightly different since same ratio \( N_S/N \) could lead to different macrostates. For ratio \( N_S/N = 0 \) and \( N_S/N = 1 \) there are no other possible microstates. But it is getting more interesting for ratio \( N_S/N = 1/7 \) (or \( N_S/N = 6/7 \)), where the same ratio \( N_S/N \) could lead to different final configuration since particle in center of the cluster will be different (it could be the smaller or the larger particle). It should have different number of contact points \( N_c \) and also different porosity \( \phi \). Possible value of \( N_S/N \) and related number of microstates for \( L = 1, 2 \) are given in table 1.

| \( L \) (\( N \))   | \( N_S/N \) (microstates) |
|---------------------|--------------------------|
| 1 (3)               | 0 (1); 1/3 (3); 2/3 (3); 1 (1) |
| 2 (7)               | 0 (1); 1/7 (1,6); 2/7 (6,6,6,3); 3/7 (6,6,3,6,6,2); 4/7 (2,6,6,6,3,6,6); 5/7 (3,6,6,6); 6/7 (6,1); 1 (1) |

Number of microstates without smaller particles in two different layers (or in a layer, ial) can be calculated using

\[ N_{ial} = C(n, k), \quad k > 1, \]  

e.g. \( N_S/N = 1/7 \) only for first microstate \( N_{ial} = 6! / (1! \cdot 5!) = 6 = (6) \), \( N_S/N = 2/7 \) after first microstate \( N_{ial} = 6! / (2! \cdot 4!) = 15 = (6+6+3) \), \( N_S/N = 3/7 \) after third microstate \( N_{ial} = 6! / (3! \cdot 3!) = 20 = (6+6+6+2) \), and the rests are similar to these. If there are particles in different layer, then possible combination should be multiplied by equation (26), e.g first row for \( N_S/N = 3/7 \) it would be obtained that \( 1 \cdot 6! / (2! \cdot 4!) = 15 = (6+6+3) \). It will be more complicated for \( L \geq 2 \).

3. Results and discussion

Number of contact points per particle is not monotonically increasing as number of layer increased. It fluctuates as shown in figure 2. Since forms of pores are similar for particle configuration with same diameter it is found that \( \phi \approx 1.43 \times 10^{-4} \) independent to \( L \). In previous work [10] the term of contactopy \( C \) is used instead of number of contact points per particles \( N_c / N \), where \( C \approx N_c/N \). From its initial configuration cluster of particles will evolve to more compact configuration as shown in figure 3. Similar results will be obtained for this work with different slopes. Final number of contact points per particle and porosity will be predicted since homogenous size of particle will again form hexagonal close packed configuration.

4. Summary

It can be summarized in this work that some programs have been developed to simulate compaction of two-dimension spherical particles as model of asteroid forming process. Number of contact points per particles fluctuates with number of layer for hexagonal close packed configuration. Porosity for three particles pairs is relatively constant.
Figure 2. Average number of contact points per particle $N_c / N$ as function of $L$.

Figure 3. Evolution of contactopy $C$ for non-homogenous particle size [10].

Acknowledgements
This work is supported by Institut Teknologi Bandung, and Ministry of Higher Education and Research, Indonesia, through the scheme Penelitian Unggulan Perguruan Tinggi – Riset Desentralisasi DIKTI in 2016 related to the vibration. Presentation of this work is supported by Committee of ISSEL 2016 and Faculty of Mathematics and Natural Sciences, Institut Teknologi Bandung.

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