Compaction of a two-dimensional system of composite spherical particles under the influence of self-gravitation: Between lock-and-key model and Tetris-structure

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Abstract. A self-gravity of spherical granular particles in the two-dimensional system is simulated. Some of the spherical particles are bonded through a spring force to form composite particles. These spherical and composite particles are attracted to each other due to gravitational force and prevented from collapse into a single point by the normal force. A previous study reported that a two-dimensional monodispersed system will form a hexagonal close-packed (HCP) configuration. In this work, it will be perturbed by some of the composite particles that could have HCP form, simple cubic (SC) form, or a mix of SC-HCP (MSH) form. These forms can be categorized into SC family (I, L, T, F, H, E), HCP family (△, O, V, X), and MSH family (⌂, K, M, W, N, Z), that can be compacted to maximum contactopy through lock-and-key mechanism (KL). The compaction of some forms from the SC family is similar to the Tetris game, where the structure should be compacted before it could be eliminated in the game. In this work, not all forms from the three families are simulated. The particles in general tend to form a final configuration with the most compact form and the composite particles seems also to influence their surrounding particles to construct the configuration.

1. Introduction
Self-gravitation is an interesting aspect in the interstellar medium, which is theoretically described as a dominant factor in constructing clouds fractal rather than turbulence [1] and has been implemented in a numerical method for investigating cloud collapse and fragmentation problem [2]. This aspect must also be also considered in modeling a planet [3], the ring of a planet [4], and materials formed on a planet [5], also its influence in the world of microscopic biology has been discussed [6]. Self-gravity of spherical particles in two-dimension has been studied for monodispersed [7] and polydispersed systems, which show that the structures evolve to form compact configuration as the contactopy value increases in time [8]. Compaction induced by two-dimensional composite particles interacting only through self-gravitation is investigated in this work. In order to form the most compact structure the composite particles move and rotate through the similar mechanism known as KL. The purpose of this work is to obtain which family (between SC and HCP) of a particle, which has a stronger influence on the surrounding of single particles.
2. Simulation
2.1. Spherical and composite particles
A spherical particle $i$ has a diameter of $D_i$ and density of $\rho_i$ will have a mass of

$$m_i = \frac{1}{6} \pi \rho D_i^3,$$

and it can have arbitrary velocity of $v_i$ with $v_i << c$ and arbitrary position of $\mathbf{r}_i$. Several spherical particles can form a composite particle, which is a cluster of particles that are bonded through a bonding force in the form of

$$\mathbf{B}_{ij} = -k_B (r_{ij} - l_{ij}) \hat{r}_{ij} - \gamma_B v_{ij},$$

between spherical particle $i$ and $j$. There are two constants in Eqn. (2), namely the binding constant $k_B$ and damping constant $\gamma_B$. The first constant will keep two particles in certain separation distance, while the second one will prevent them from oscillating during changing positions. The term $r_{ij}$ stands for the distance between particle $i$ and $j$, while $l_{ij}$ stands for a normal distance between the two particles. It is a distance when the force is zero. If particle $i$ is in a position of $\mathbf{r}_i$ and particle $j$ in a position of $\mathbf{r}_j$, then their relative position will be

$$\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j,$$

the distance between the particle

$$r_{ij} = |\mathbf{r}_{ij}| = \sqrt{\mathbf{r}_{ij} \cdot \mathbf{r}_{ij}},$$

and its related unit vector

$$\hat{r}_{ij} = \frac{\mathbf{r}_{ij}}{r_{ij}}.$$

Relative velocity $v_{ij}$ in Eqn. (2) can be obtained using a similar way as obtaining $\mathbf{r}_{ij}$ in Eqn. (3).

![FIGURE 1. Families of composite particles: Example of the composite particles (top) and example of key-lock pair (bottom) in each family. Each family is assigned to different colors (red for S-family, green for M-family, blue for H-family).](image-url)
There are three families of composite particles. The first is S-family where the particles form a simple cubic (SC) arrangement, the second is H-family where the particles form a hexagonal close-packed (HCP) arrangement, and the last is M-family where there is a mixture between SC and HCP arrangements. In this work, it is limited only to the two-dimensional system as shown in Fig. 1.

In the top row of Fig. 1, there are examples of composite particles for all family, while in the bottom row examples of key-lock pairs are given. Special key-lock pair in S-family, which already very familiar in the Tetris game, still requires the most suitable optimization method [9] and how the game works can be used in the deposition process at the nanoscale [10]. There are two different value of nearest neighbor normal distance $L_{ij}$, which are

$$L_{ij} = \begin{cases} D_i, & r_y = \frac{1}{2} (D_i + D_j), \\ \sqrt{2D}, & r_y > \frac{1}{2} (D_i + D_j). \end{cases} \quad (6)$$

that hold only for monodispersed system or $D_i = D_j$. A composite particle in H-family will have only the second value, while the other two-families will have both values. Value of $l_{ij}$ in Eqn. (2) can be $L_{ij}$ or other values that could be simply a linear combination of $L_{ij}$ or more complicated value.

![FIGURE 2. Illustration of $l_{ij}$ value in S-, M-, and H-families, that could be $L_{ij}$ or its linear combination: first $L_{ij}$ (black solid line) second $L_{ij}$ (black dashed line), and its linear combination (purple dotted line).](image)

Values of $l_{ij}$ in Fig. 2 are $L_{ij}$ for S-family, $L_{ij}$ and other value for M- and H-families. These other values can be obtained using simple trigonometry, where it could be

$$l_{ij}^{mn} = D \sqrt{n^2 + m^2} \quad (7)$$

with $m, n = 1, 2, \ldots$, for S-family,

$$l_{ij}^m = Dn \quad (8)$$

with $m, n = 1, 2, \ldots$, for S- and H-families, and

$$l_{ij}^{nm} = D \sqrt{n^2 + \left(\frac{1}{2}m\right)^2} \quad (9)$$

for other values. But since the binding force in Eqn. (2) only for nearest neighbor particle or at least one particle after the nearest neighbor, we are interested only in smaller values of $m$ and $n$. 

3
2.2. Interaction forces

Two types of interaction forces between spherical particles are considered in this work. The former is an attractive force in the form of gravitation force and the later is a repulsion force in the form of a limited-range spring force using a linear spring-dashpot model [11]. The attraction force is formulated as

$$
\tilde{G}_{ij} = -k_G \frac{m_i m_j}{r_{ij}^2} \hat{r}_{ij},
$$

(10)

with \( m_i \) and \( m_j \) are mass of particle \( i \) and \( j \), and \( k_G \) is universal gravitation constant, which will use artificial value in this work. And the repulsion force is formulated as

$$
\tilde{N}_{ij} = k_N \xi_{ij} \hat{r}_{ij} - \gamma_N \xi_{ij} \hat{v}_{ij},
$$

(11)

with \( k_N \) and \( \gamma_N \) are spring and damping constants in the linear spring-dashpot model. Eqn. (11) will hold only for limited range, which is defined by the overlap

$$
\xi_{ij} = \max \left[ 0, \frac{1}{2} (D_i + D_j) - r_{ij} \right],
$$

(12)

with

$$
\max(a, b) = \begin{cases} a, & a \geq b, \\ b, & a < b, \end{cases}
$$

(13)

and

$$
\hat{\xi}_{ij} = -\hat{v}_{ij},
$$

(15)

Forces in Eqns. (10) and (11) hold for individual spherical particles and also for the composite particles.

2.3. Numerical method

At time \( t \) sum of all forces acted upon a particle \( i \) is

$$
\sum \tilde{F} = \sum_j \tilde{B}_j + \sum_k \tilde{N}_k + \sum_l \tilde{G}_l,
$$

(16)

where \( j \) is only in a composite particle, \( k \) is only between two composite particles, and \( l \) is for all particles. Details on how to limit the indices \( j \) and \( k \) will not be shown here since it is too technical to discuss. From Newton’s 2nd law of motion, it can be obtained that

$$
\tilde{a}_i(t) = \frac{1}{m_i} \left( \sum_j \tilde{B}_j + \sum_k \tilde{N}_k + \sum_l \tilde{G}_l \right).
$$

(17)

In general \( \tilde{B}_j = \tilde{B}_j(\tilde{r}_1, \ldots, \tilde{r}_i, \ldots, \tilde{r}_N, \tilde{v}_1, \ldots, \tilde{v}_i, \ldots, \tilde{v}_N) \) and also for \( \tilde{N}_{ij} \) and \( \tilde{G}_{ij} \), which means that acceleration of particle \( i \) is due to the position and velocity of other particles in the system. Using the simplest numerical method, it can be obtained that

$$
\tilde{v}_i(t + \Delta t) = \tilde{v}_i(t) + \tilde{a}_i(t) \Delta t
$$

(18)

and

$$
\tilde{r}_i(t + \Delta t) = \tilde{r}_i(t) + \tilde{v}_i(t) \Delta t.
$$

(19)
After obtaining a new value of position and velocity of all particles, these values can be used to calculate new acceleration in Eqn. (17). Repeating this process using Eqns. (16) – (19) will give the dynamics of all particles.

2.4. Analysis
Using Eqn. (12) in the form of

\[ C = \sum_{i=1}^{N} \sum_{j=1}^{N} \text{sign}(\xi_{ij}), \]  

contactopy \( C \) of the system, which can be calculated for the whole system consists of \( N \) spherical particles [12], is used for composite particles in this work. The distribution of nearest neighbor distance \( \lambda \) from the same previous work will also be used, which is limited from 0 to \( \sqrt{2} D \). For a perfect S-family system there will be only two values, which are \( D \) and \( \sqrt{2} D \). The first value is for two spherical particles in contact and the second value is for two spherical particles in opposite corners of an SC two-dimensional lattice. Meanwhile, for a perfect H-family, there is only one value, \( D \). Between the values 0 and \( \sqrt{2} D \) there will be about 20 classes in order to make the distribution.

3. Results and discussion
Table 1 shows the values of parameters used in the simulation, where all values are in SI unit. There is no parameter variation conducted in the simulation, but only the forms of composite particles, where we can not yet define parameters related to the forms.

| Parameter | Value | Unit |
|-----------|-------|------|
| \( D \)   | 0.1   | m    |
| \( \rho \) | 500   | kg/m³|
| \( N \)   | 100   | –    |
| \( k_N \) | 1000  | N/m  |
| \( \gamma_N \) | 0.1 | kg/s |
| \( k_S \) | 1000  | N/m  |
| \( \gamma_S \) | 10  | kg/s |
| \( m^2k_G \) | 0.01 | N/m² |
| \( \Delta t \) | \( 5 \times 10^{-3} \) | s    |
| \( T_{data} \) | 1     | s    |

During the structure evolution, a particle and a composite particle can penetrate into space between two particles or composite particles due to self-gravitation interaction among all particles (and composite particles). This mechanism is similar to the system of three frictionless spherical grains [13] or a pile of cylindrical particles [14], where both are under the influence of earth gravitation.

Four initial configurations are first tested to investigate the role of a composite particle in changing its environment particles (gray circles). One type of composite particles from each S- and H-families are used. From S-family a 2×2 composite particle (red circles) is chosen and from H-family also 2×2 composite particle (blue circles) is chosen.
FIGURE 3. Evolution of a 10×10 two-dimensional particle configuration with the bed of spherical particles, which are (a) without composite particles, (b) with composite particles from S-family, (c) with composite particles from H-family, and (d) with composite particles from S- and H-families.

The first configuration in Fig 3(a) shows only the bed particles that will form an HCP configuration due to their self-gravitation interactions. The existence of composite particles from S-family could affect its environment and prevent the bed particles in forming HSC configuration, at least the particles between the composite particles as shown in Fig. 3(b). Introducing a composite particle from H-family does not give an interesting final results since an HCP is already a favorite configuration, except that a composite particle from this family could have different internal compaction compared to the bed particles, which will produce another peak in the nearest neighbor distance $\lambda$ distribution as Fig. 3(c) shows. By introducing composite particles from each family to the system at each side of the system, it is obtained that the influence of H-family will override the influence of S-family as given by Fig. 3(d).

Composite particles produced in this work can be further used to simulate another more complex system, e.g. orientation of semolina seeds in static electric field [15], where the interaction between seeds is similar to Eqn. (10), but with the absence of normal force in Eqn. (11), due to the viscosity of surrounding fluid (castor oil), that makes the composite particles will be only rotated but not moved due to the electric field. The seed itself is simply the form of S-family composite particles with linear form ($N \geq 2$). Beside the mentioned implementation, another aspect that can be deeper investigated in the future is the detail of KL mechanism, such as how long a compaction takes time from different initial configurations, how many final configuration can be constructed from similar initial configurations, or how many initial configurations can evolve to the same final configuration. These questions are interesting to answer.

4. Conclusion
Simulation of compaction of a two-dimensional system of composite spherical particles under the influence of self-gravitation for 100 particles has been performed. The result shows that the existence of S-family composite particles can affect their neighbor configuration, but it will be overridden by the
existence of H-family composite particles. H-family of particle has a stronger influence on its surrounding particles compared to S-Family.

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