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Dense packing of general-shaped particles using analytical and minimization techniques

Empaquetamiento denso de partículas de forma general usando técnicas analíticas y de minimización

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Abstract

The Discrete Element Method (DEM) is a numerical method that has achieved general acceptance as an alternative tool to model discontinuous media, with a wide range of practical applications. Given that spheres are not always a suitable shape for DEM simulations, other particle shapes need to be used. However, for shapes different from spheres, there are not many advancing front packing algorithms, which are, in many cases, the best algorithms that allow obtaining an appropriate initial set of particles for a DEM simulation. This lack of advancing front packing algorithms for shapes different from spheres is mostly due to the difficulty of solving the problem of placing a mobile particle in contact with other two (in 2D) or three (in 3D) particles. In this paper, new methods for solving the problem of the particle in contact are proposed. First, the problem of the particle in contact is formally defined. In the case of the wrappers solution method, it is applied to geometrical shapes to which has not been applied before. In the case of the minimization method, which is an original creation of the authors, it is shown to be a promising alternative for spherocylinders.

Keywords: *DEM; packing, particle in contact; optimization; spherocylinders*

Resumen

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El Método de Elementos Discretos (MED) es un método numérico que ha alcanzado una gran aceptación como herramienta alternativa para modelar medios discontinuos, con un ampllio rango de aplicaciones prácticas. Dado que las esferas no son siempre apropiadas para simulaciones con el MED, es necesario usar otras formas de partícula. Sin embargo, para formas diferentes de las esferas, no se dispone de muchos algoritmos de empaquetamiento de avance frontal, los cuales son, en muchos casos, los mejores algoritmos que permiten obtener un conjunto inicial de partículas apropiado para una simulación con el MED. Esta falta de algoritmos de avance frontal para formas no esféricas se debe principalmente a la dificultad de resolver el problema de colocar una partícula móvil en contacto con otras dos (en 2D) o tres (en 3D) partículas. En este artículo son propuestos nuevos métodos para resolver el problema de la partícula en contacto. Primero, el problema de la partícula en contacto es formalmente definido. En el caso de la solución con envolventes, esta es aplicada a formas a las cuales no había sido aplicado antes. En el caso del método de minimización, el cual es una creación original de los autores, se muestra que es una alternativa promisoria para esferocilindros.

Palabras clave: MED, empaquetamiento, partícula en contacto, optimización, esferocilindros

Introduction

The Discrete Element Method (DEM) is a numerical method that has achieved great recognition as an alternative tool to model discontinuous media. Several professional (2014, ITASCA Consulting Group 2014) and free software (Smilauer, Catalano et al. 2010) are available for this purpose. Practical applications to a wide range of problems may be found in the recent literature (Catalano, Chareyre et al. 2014, Lim and Andrade 2014); however most of them assume spherical particles. Spheres are simple to code and easy to use, but in many cases they cannot capture the basic dynamic mechanisms and therefore do not provide the most adequate geometric model for the particles. For instance, an individual disc (or sphere) will always roll down over a rough slope; however, a generic particle, such as a cluster of disks, may stay in static equilibrium, slide or roll, depending on the slope angle, the tangential friction coefficient and the particle shape (Mohammadi). Particle types other than disks or spheres used in DEM include: clusters of spheres, which enable to model a wide range of different shapes, polyhedra, ellipses and ellipsoids, superquadrics and spherocylinders, among others.

When DEM began to be applied some years ago, one of its major problems was the cost of obtaining an initial set of particles with a high volume (area) fraction, which is defined as the ratio of solid volume (area) to the total volume (area). Most of the initial applications used some kind of dynamic algorithm, in which a loose packing of non-overlapping particles is generated at random positions, and later the particles are rearranged by imposing some loading

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and boundary conditions (Cheng, Guo et al. , Jia and Williams , Han, Feng et al. , Mueller , Fraige, Langston et al.). Dynamic algorithms are computationally costly because they require a previous DEM simulation. Hence it was necessary to develop constructive packing methods, which are characterized by the sequential placement of particles at their final positions (Feng, Han et al. 2002, Feng, Han et al. 2003, Löhner and Oñate 2004, Bagi 2005, Benabbou, Borouchaki et al. 2010, Pérez Morales, Pérez Brito et al. 2010, Pérez Morales, Roselló Valera et al. 2011, Valera, Morales et al. 2015). The class of constructive methods includes "advancing front algorithms".

An advancing front is a group of particles in the surroundings of the evolving system of particles under generation. A group of previously placed particles lie inside the advancing front, while new particles are placed in contact with the outer particles of the front. The packing usually starts with a set of two or three particles at any given position, or one or two particles in contact with the walls defining the domain (walls are also considered particles in this context). These particles comprise the initial advancing front. Then a new particle is generated or chosen from a repertory of particles to be added to the packing. Next, the new particle is placed at a position that just touches other particles in the advancing front. Then the advancing front is updated and the process continues. Pseudocode 1 summarizes the basic steps of a generic advancing front algorithm (Feng, Han et al.).

1. Initialize the packing (usually with two or three particles).
2. Generate or select the particle to be packed.
3. Select an active front and determine the position at which the particle just touches the particles in the front.
4. Check if the particle at this position overlaps with any existing particles.
5. If no overlap occurs, accept the new particle and return to step 2 for the next particle. Otherwise go to step 6.
6. Reject the position and repeat step 3 for another active front.

Pseudocode 1. General steps that are common to all advancing front packing algorithms.

In order to carry out step 3 of Pseudocode 1, the problem of placing a particle in contact with others must be solved (see section 3). In this sense, some authors state that a higher local density is achieved if each new particle added to the media is placed in contact with other two existing particles in the two-dimensional (2D) case (Feng, Han et al.). In the analogous three-dimensional (3D) case, the contact involves other three existing particles. For spherical particles of equal size, Kepler's conjecture (Weisstein) is the solution for a maximum global volume fraction. Apollonius circle problem (Weisstein) is also related to placing particles in contact, but it is not exactly the problem that is solved further in this paper using minimization.

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The problem of placing a particle in contact with other two (in 2D) or other three (in 3D) fixed particles has been solved using a direct approach, for some types of particles, as part of advancing front packing algorithms. Such direct approach is briefly explained in section 3.1, and the types of particles mentioned above are circles (Feng, Han et al. 2003, Bagi 2005), polygons (Feng, Han et al. 2002), ellipses (Feng, Han et al. 2002) and spheres (Benabbou, Borouchaki et al. 2009). The solution of the problem can be not unique, as will be seen in section 3.

Even for simple shapes such as ellipses, the previously mentioned direct approach can be very difficult to apply, given the complexity of the analytical expressions that have to be obtained. That is why an alternative procedure based on minimization is presented in section 3.2, together with a comparison with the direct approach when possible.

Optimization techniques have been used as an auxiliary tool in the process of packing particles for DEM. For example, the position and dimension of particles can be modified iteratively in order to decrease the empty space in the domain, and in order to eliminate the gap between the domain boundary and the particles (Labra and Oñate 2008). Also, the remaining heterogeneities in the packing can be removed, even without modifying the shape or dimensions of particles (Benabbou, Borouchaki et al. 2010). However, to the best of the authors' knowledge, optimization has never been used before by other researchers in order to place a particle in contact with other two (in 2D) or other three (in 3D) fixed particles.

Construction of a particle in contact with others

Let $p[\mathbf{c}]$ denote a particle in $\mathbb{R}^n$ such that $\mathbf{c} \in \mathbb{R}^n$ is a point with the property that any rotation or translation applied to $p[\mathbf{c}]$ must also be applied to $\mathbf{c}$ and vice versa. Now consider the following problem:

Placing a particle in contact with others

Let $p_1, \dots, p_n$ be n fixed particles in $\mathbb{R}^n$ ($n \in \{2,3\}$), and let $p_{mob}[\mathbf{c}]$ be another particle that must be translated, without making rotations, in such a way that $p_{mob}[\mathbf{c}]$ be in outer contact with all the particles p_i simultaneously, $i = \overline{1,n}$, without overlapping with any of them. Find the points $\mathbf{c}$ that satisfy this condition. From now on, particle $p_{mob}[\mathbf{c}]$ will be referred to as the "mobile particle", in order to simplify the terminology, despite it is not actually moving. The phrase "without making rotations" can be better understood by looking at Figure 1(a). The mobile particle there, $p_{mob}[\mathbf{c}]$, changes its position but preserves its inclination, in such a way that it is not rotated.

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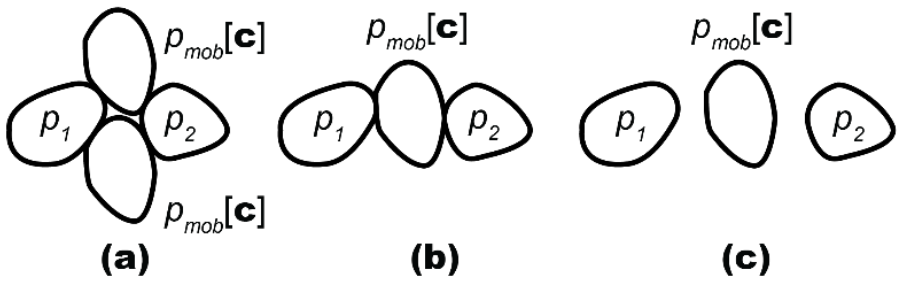

Figure 1. Number of solutions for the problem of placing a particle in contact with others.

It has been verified in practice that in the general case, the problem of placing a particle in contact with others has at most two solutions when particles $p_1, \dots, p_n$ and $p_{mob}[\mathbf{c}]$ are convex and are close enough to each other (Figure 1(a)). This can degenerate to only one solution when the mobile particle fits exactly in the gap between the fixed particles (Figure 1(b)). Obviously, there is no solution when $p_1, \dots, p_n$ are apart from each other by a distance greater than the larger Feret dimension of the particle to be placed (Figure 1(c)).

In the case of spherical particles and clusters of spheres it is possible to develop an analytical solution for the problem proposed above based on the concept of wrapper's intersection (Hernández Ortega 2003, Benabbou, Borouchaki et al. 2010, Pérez Morales 2012), explained in the following section 3.1. However the analytical procedures may become too cumbersome in the case of polyhedra and there is no analytical solution for particles with general shape. An alternative methodology that may be eventually generalized for these cases is explored in section 3.2. The two solutions are compared when possible.

Wrappers intersection method for placing a particle in contact with others

Let p_{fix} be a fixed particle and $p_{mob}[\mathbf{c}]$ be a mobile particle. The locus defined by all points $\mathbf{c}$ such that p_{fix} and $p_{mob}[\mathbf{c}]$ are in outer contact, will be called *wrapper*.

In two dimensions, if the fixed and mobile particles are circles with radii equal to r_{fix} and r_{mob} respectively, then the corresponding wrapper is obviously a circle with radius $r_{fix} + r_{mob}$. When the two particles are described by polygons, the wrapper is a polygon with twice the number of sides of the fixed one. In the case of mixed particles, a circle and a polygon, the resulting wrapper is a polygon with rounded corners. Similar geometries are generated in the three dimensional case.

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The method of wrappers intersection in $\mathbb{R}^n$, for translating a mobile particle $p_{mob}[\mathbf{c}]$ in such a way that it is in outer contact with other fixed particles $p_1, \ldots, p_n$, without overlapping, consists of finding the loci described by $\mathbf{c}$ when sliding $p_{mob}[\mathbf{c}]$ around each of the fixed particles, then finding the intersections of these loci, and finally translating $\mathbf{c}$ to make it coincide with these intersections. For convex particles in 2D, the number of these intersections should be equal to two in the general case, equal to one in the degenerate case, or equal to zero in the case of no solution. It is important to notice that the choice of $\mathbf{c}$ is irrelevant as long as its position remains unchanged with respect to the mobile particle.

The wrappers intersection method has previously been applied to shapes such as circles (this case can be solved using a formula for finding the intersection of two circles (Wang and Liang 1997)), ellipses (Wang and Liang 1997, Feng, Han et al. 2002), polygons (Feng, Han et al. 2002) and spheres (Hernández Ortega 2003, Benabbou, Borouchaki et al. 2009). Here it is shown how to apply this method to other shapes such as clusters of circles, mixes of polygons and circles, spheres (by a different way than (Hernández Ortega 2003, Benabbou, Borouchaki et al. 2009)), clusters of spheres and convex polyhedra.

Circles

Circles are perhaps the easiest shape for which the wrappers intersection method can be used. Let C_1 and C_2 be two circles with centers $\mathbf{c_1}$ and $\mathbf{c_2}$ and radii r_1 and r_2, respectively. Let $C_{mob}[\mathbf{c}]$ be a mobile circle of center $\mathbf{c}$ and radius r_{mob}, to be placed in outer contact with C_1 and C_2 simultaneously. The wrappers formed by sliding $C_{mob}[\mathbf{c}]$ around C_1 and C_2 are the circles C'_1 and C'_2 with the same centers than C_1 and C_2 and radii $r_1 + r_{mob}$ and $r_2 + r_{mob}$, respectively. If C_{31} and C_{32} are the circles obtained by centering $C_{mob}[\mathbf{c}]$ at the two intersection points of C_1 and C_2 (in case they exist), then C_{31} and C_{32} are in outer tangency with C_1 and C_2 simultaneously. The formula for finding such intersection points can be found at (Wang and Liang 1997).

Clusters of circles and clusters of spheres

Now consider the case at which p_1, p_2 and $p_{mob}[\mathbf{c}]$ are clusters of circles. Due to the difficulty of explicitly representing the wrappers, the method here will be different. Instead of a general formulation, an example with three composite particles, each one formed by a cluster of only two circles, will be used for a better understanding.

Let $\mathbf{c_{ij}}$ (r_{ij}) be the center (radius) of the *j*-th circle comprising the *i*-th particle. It can be seen in Figure 2 that the composite particle $p_3 = p_{mob}[\mathbf{x}]$ has been placed by a translation $\mathbf{x}$ of $p_{mob}[\mathbf{x}]$ in such a way that it is in outer contact with composite particles p_1 and p_2 simultaneously.

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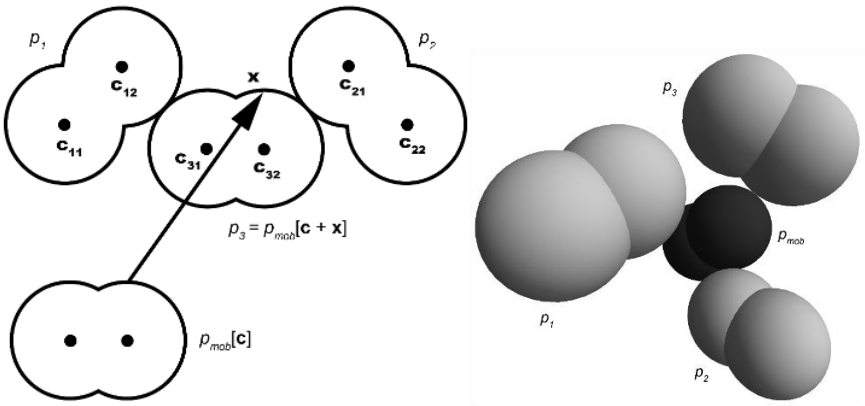

Figure 2. Left: particle $p_{mob}[\mathbf{c}]$ is translated in such a way that it is in contact with p_1 and p_2 simultaneously. Right: Cluster of spheres in contact with other three.

It can also be seen that the contact between particles p_1 and p_3 occurs between circle 2 of p_1 and circle 1 of p_3, and that the contact between particles p_2 and p_3 occurs between circle 1 of p_2 and circle 2 of p_3. Knowing this beforehand and denoting by $\mathbf{x}$ the translation that puts $p_{mob}[\mathbf{c}]$ in contact with p_1 and p_2 simultaneously, this translation can be found by solving the following system:

$$\|\mathbf{x} + \mathbf{c_{31}} - \mathbf{c_{12}}\|^2 = (r_{12} + r_{31})^2 \quad (1)$$

$$\|\mathbf{x} + \mathbf{c_{32}} - \mathbf{c_{21}}\|^2 = (r_{21} + r_{32})^2 \quad (2)$$

where $\|\ \ \|$ denotes the Euclidean norm of a vector. Equations (1) and (2) form a system with two unknowns, the coordinates of vector $\mathbf{x}$. The solution is the same as the intersection of two circles centered at points $\mathbf{c_{12}} - \mathbf{c_{31}}$ and $\mathbf{c_{21}} - \mathbf{c_{32}}$ with radii equal to $r_{12} + r_{31}$ and $r_{21} + r_{32}$, respectively, and can be calculated in a straightforward manner (Wang and Liang 1997).

Given that in practice it is not possible to know beforehand between which circles the contacts will take place, it is necessary to verify, in the worst case, all the possible combinations of circles comprising each pair of clusters, discarding solutions for which the translated particle overlaps with some of the fixed ones. The time for performing all these checks has an order of time $O(n_1 n_2 n_3^2)$, where n_1, n_2 and n_3 are the number of circles comprising the fixed and mobile particles respectively. In practice, calculations can be stopped when two solutions are obtained. The procedure for constructing a cluster of spheres in contact with other three composite particles (Figure 2 right) is analogous to the case of clusters of circles, so details will not be given.

Combination of different particle shapes: mix of circles and polygons

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A possible case of application of the wrappers intersection method in $\mathbb{R}^2$ is when p_1, p_2 and $p_{mob}[\mathbf{c}]$ can be circles or convex polygons. The wrappers obtained here are circles, polygons, or circumpolygons, which are formed by line segments and arcs of circles interleaved. A circumpolygon can be obtained when sliding a mobile circle around a fixed polygon or vice versa.

Finally, the intersection of two circumpolygons is reduced to finding intersections between sets of line segments and arcs of circles. A search should be made to test the intersections between all segments and arcs defining each wrapper (circumpolygon). An example of a mobile circle placed in contact with a fixed circle and a fixed polygon, as well as a packing of circles and polygons, can be seen at **¡Error! No se encuentra el origen de la referencia.**. The area fraction and coordination number of such packing are equal to 0,69 and 3,98 respectively.

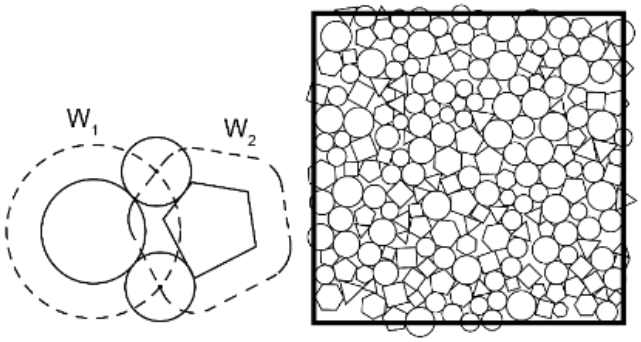

Figure 3. Left: mobile circle centered at the intersection of the wrapper circumpolygons. Right: packing of circles and polygons.

Polyhedra

The wrappers intersection method has a high computational cost when applied to polyhedra. When sliding a mobile polyhedron around a fixed one, the obtained wrapper is another more complex polyhedron, whose shape is determined by that of the fixed and mobile polyhedra. The number of faces of the wrapping polyhedron is equal to the sum of the number of faces, edges and vertices of the fixed polyhedron.

The faces of the wrapping polyhedron can be obtained in the following ways:

1) Sliding mobile vertices over fixed faces (Figure 4 left).
2) Sliding mobile faces over fixed vertices (Figure 4 center).
3) Sliding mobile edges over fixed edges (Figure 4 right).

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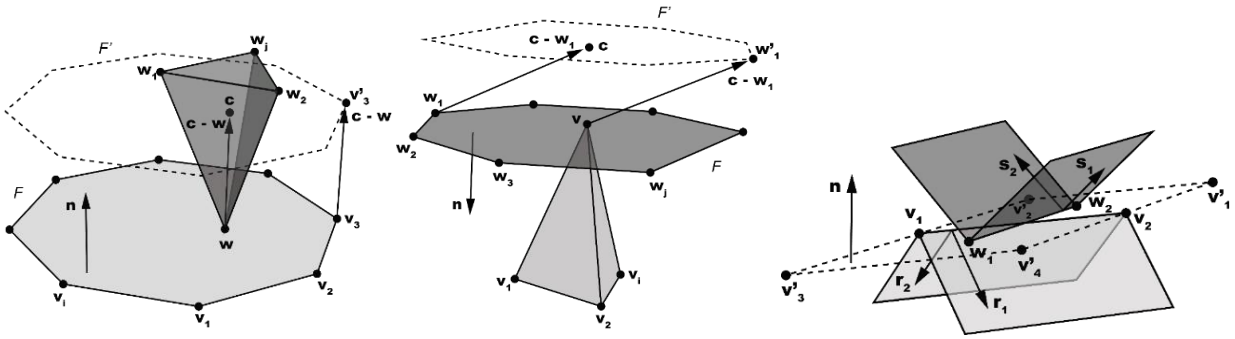

Figure 4. Left: Slide of a mobile vertex **w** over a fixed face F. Center: Slide of a mobile face F over a fixed vertex **v**. Right: Slide of a mobile edge $\overline{\mathbf{w_1 w_2}}$ over a fixed edge $\overline{\mathbf{v_1 v_2}}$.

When carrying out each of the previous steps, the center of mass **c** of the mobile polyhedron describes a polygon which is a face of the wrapper polyhedron.

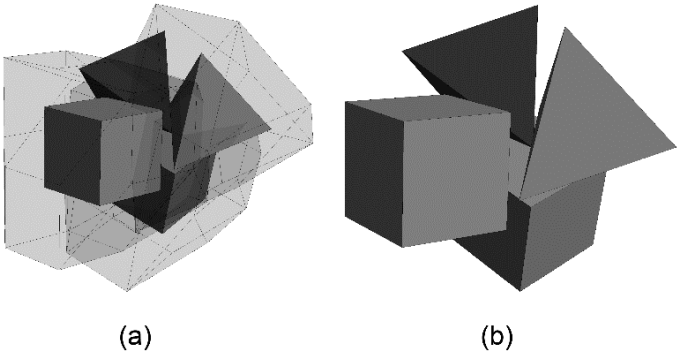

Figure 5. Example of wrappers intersection with polyhedra. (a) Fixed polyhedra, wrappers and mobile polyhedron placed at one of the two intersection points of the three wrappers. (b) The same as (a) without the wrappers. The mobile polyhedron is in outer contact with the three fixed polyhedra.

Figure 5 shows the process of placing a polyhedron in contact with other three, translated according to the previous formulations.

Potential minimization method for placing a particle in contact with others

The method corresponding to this section uses an optimization approach to solve the problem of the particle in contact. In some cases, it can be easier to apply than wrappers intersection because it only requires the definition of a continuous function $\omega(p_1, p_2)$ for a pair of particles (p_1, p_2) such that:

$$\omega(p_1,\ p_2)\begin{cases}\leq 0\ if\ p_1 \cap p_2 \neq \emptyset \\ > 0\ otherwise\end{cases} \quad (3)$$

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Function $\omega(p_1,\ p_2)$ is a measure of the gap between the surfaces of the two particles. Condition (3) implies that p_1 and p_2 are in outer contact without overlapping if and only if $\omega(p_1,\ p_2) = 0$. Function ω is usually not unique. Explicit formulas for function $\omega(p_1,\ p_2)$ will be given in next sections for the cases of disks, spheres and spherocylinders.

Once the gap function ω has been chosen, the solution to the problem of placing a particle in contact with others can be obtained by solving the following optimization problem:

$$\begin{array}{ll} minimize & |\omega(p_1, p_{mob}[\mathbf{x}])| + \cdots + |\omega(p_n, p_{mob}[\mathbf{x}])| \\ subject\ to & \mathbf{x} \in \mathbb{R}^n \end{array} \quad (4)$$

Condition (4) means that a particle is in simultaneous outer contact with other two particles in 2D (or three in 3D) when the sum of the gaps is minimized (in this case the minimum should be zero). Since two solutions for problem (4) are being searched in most cases (see Figure 1), such problem has to be solved twice each time in practice, with an additional restriction that indicates which solution is being searched. Such restriction is based on the fact that the centers of the two solution particles usually lie on different half-spaces defined by the centers of the fixed particles. In the 2D case, the half-spaces are the half-planes determined by the line joining the centers of the two fixed particles, while in the 3D case the half-spaces are determined by the plane containing the centers of the three fixed particles. In order to solve the minimization problem the authors used the Nelder-Mead method (Nelder and Mead 1965) already validated and included in a commercial software for the 2D cases, and the same method available in a free C++ library (2015), for the 3D cases. This method was initially chosen because it requires relatively few evaluations to reach the global minimum, and does not require derivative information of the objective function.

Circles or spheres

For any two circles or spheres p_1 and p_2, $\omega(p_1, p_2)$ can be defined by the equality

$$\omega(p_1, p_2) = \|\mathbf{c_1} - \mathbf{c_2}\|^2 - (r_1 + r_2)^2 \quad (5)$$

where $\mathbf{c_1}$ and $\mathbf{c_2}$ are the coordinates of centers of the particles and r_1 and r_2 their radii, respectively. It is possible to verify that expression (5) satisfies (3).

Spherocylinders

A spherocylinder is a capsule-like body determined by a line segment and a positive real number called radius, and is defined as the set of all points that lie at a distance from the segment equal to or smaller than the radius. For this type of particle, the potential minimization method is perhaps the most suitable in order to build the particle in contact. If p_1

and p_2 are two spherocylinders defined by segments $\boldsymbol{s_1}$ and $\boldsymbol{s_2}$, and radii r_1 and r_2 respectively, then the function $\omega(p_1, p_2)$ can be defined by the following equality:

$$\omega(p_1, p_2) = d_1(\boldsymbol{s_1}, \boldsymbol{s_2})^2 - (r_1 + r_2)^2 \quad (6)$$

where $d_1(\boldsymbol{s_1}, \boldsymbol{s_2}) = \inf\{d(\boldsymbol{\lambda_1}, \boldsymbol{\lambda_2}): \boldsymbol{\lambda_1} \in \boldsymbol{s_1}, \boldsymbol{\lambda_2} \in \boldsymbol{s_2}\}$ is the distance between segments $\boldsymbol{s_1}$ and $\boldsymbol{s_2}$ (a procedure for calculating the distance between two line segments can be seen in (Eberly 2015)), being d the usual distance in $\mathbb{R}^n$.

Given that for spherocylinders the wrappers were very complicated to describe, especially in 3D, a preliminary comparison in 2D between wrappers and minimization (Figure 6 left) was carried out by approximating spherocylinders with clusters of 4 disks each in the case of wrappers. In (Löhner and Oñate 2004) the reader can find approximations of some simple shapes with clusters. A packing of spherocylinders in 3D was also obtained (Figure 6 right).

The two packings can be seen in Figure 6 left. In both packings, contained in squares of side equal to 20 units, the particles have an aspect ratio equal to 0,5, and circumscribed radii following the $U[1, 2]$ distribution. The packing of 73 clusters (Figure 6 left (a)), obtained by wrappers intersection, was generated at a speed of 1,05 particles per second, while the packing of 77 spherocylinders (Figure 6 left (b)) obtained by minimization, was generated at a speed of 0,0094 particles per second. This suggests that if generation of spherocylinders using wrappers was possible, it would be by far faster than generation using minimization. However, as was already mentioned, the formulation of wrappers intersection for spherocylinders, especially in 3D, is not a trivial task. The area fractions of the packings were equal to 77,21% and 82,20% for the cases of Figure 6 left (a) and Figure 6 left (b), respectively.

The packing of spherocylinders generated in 3D can be seen in Figure 6(b). It comprises 5901 particles generated at a speed of 3,90 particles per second, and is contained within a cube of side equal to 40 units. This speed is so much higher than the analogous speed in 2D, because in this case an efficient implementation in C++ was used. Each particle has an aspect ratio of 0,5, and the circumscribed radii of the particles follow the $U[1,2]$ distribution. The volume fraction of the packing, measured with respect to the circumscribed box, is equal to 45,77%.

For the sake of comparison, another packing of 4778 spherocylinders approximated with clusters was generated (Figure 6(a)). Given that in this case the generation speed with wrappers was very slow, an approximate wrappers method was implemented, producing a packing with a much less volume fraction equal to 36,68%, but generated at the convenient speed of 172,30 particles per second. This packing is also contained in a cube of side equal to 40 units. It is interesting that not only in this case, but also in all packings presented in this paper, the volume fraction of packings obtained with minimization is higher than the volume fraction of analogous packings obtained using wrappers.

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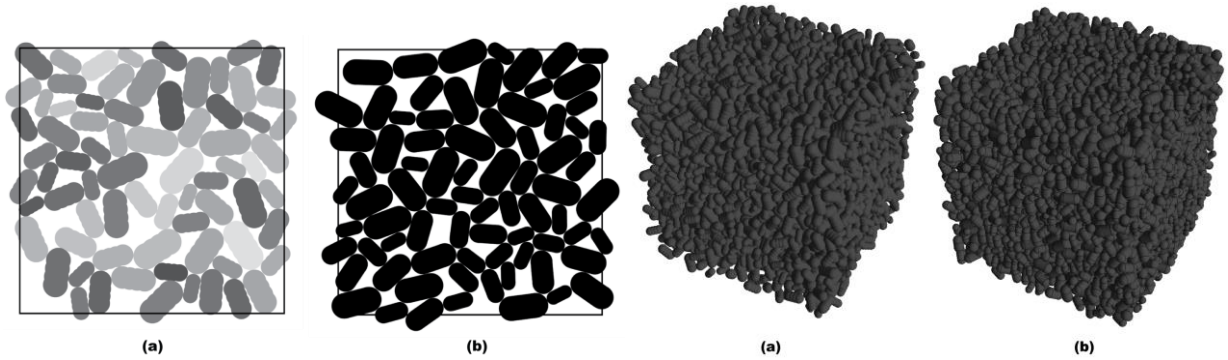

Figure 6. **Left:** Comparison between wrappers and minimization in 2D spherocylinders. (a) packing of spherocylinders approximated with clusters of disks and generated with wrappers intersection; (b) packing of spherocylinders generated with minimization. **Right:** comparison between wrappers and minimization in 3D spherocylinders. (a) Packing of 4778 spherocylinders approximated with clusters; (b) Packing of 5901 spherocylinders generated with minimization.

Conclusion

The problem of placing a mobile particle in contact with other two (in 2D) or three (in 3D), as part of advancing front particle packing algorithms in the context of DEM simulations, has been little studied in the available literature. The geometric solution of such problem only exists for a few particle shapes, and is only based on the direct approach. In this paper, the existing solution method has been applied to cases in which it had not been used. Moreover, a new solution method, based on minimization has been proposed. This new method was shown to be a promising alternative for packing spherocylinders.

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