# Realistic Generation and Packing of DEM Sand Samples

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## ABSTRACT

This paper presents a novel method of generating and packing realistic sand samples for discrete element modeling. In order to generate an assembly of 2D particles in an arbitrary container shape, a number of essential properties are identified and reproduced, including size distribution, packing density, possible preferred particle orientation, and particle shapes. Four descriptors (Elongation, Circularity, Roundness and Regularity) are considered to characterize these shape factors.

To generate the packing, the container is partitioned into a number of polygons using a Constrained Voronoi Tessellation with prescribed statistical distribution of the polygons sizes and orientations. An iterative stochastic method is employed to perform the tessellation. Each polygon of the tessellation is then filled with a virtual sand particle, generated randomly and accordingly to the prescribed shape features. A method based on the discrete Fourier transform is used for the generation. Finally, each virtual particle is replaced by a collection of discs, also called Overlapping Discrete Element Clusters (ODECs). The whole packing is then ready for use in a DEM simulation.

The proposed method has been applied to the modeling of repose angle of Toyoura sand in comparison with experimental results. The process of calibration of the contact laws in the DEM simulation is discussed, and the potential of the method in a broad field of applications is highlighted.

## 1. INTRODUCTION

Understanding the micromechanical behaviour of granular materials has become a major thematic topic in several scientific fields, such as geomechanics, powder industry, or sedimentology. While modern experimental techniques provide an insight into the small-scale behaviour of granular materials (Desrues et al. 2004, Hall et al. 2010, Cavaretta et al. 2010), the continuous increase of computational power has led to a growing interest in numerical simulation of granular behavior based on a discrete modelling of the grain scale of granular media.

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The Discrete Elements Method (DEM) was first proposed by Cundall and Strack (1979), and has been continuously developed and improved over the past decades. One of the most recent challenges in such simulations is to account for the realistic shapes of the particles. In the field of geomechanics, for example, natural sands may have very different intrinsic properties, depending on their geological history and mineralogical composition (Blott and Pye 2008). This kind of property is expected to have a large influence on the mechanical behaviour of these sands, and the discrete methods are certainly a relevant way to investigate this influence. While the majority of discrete simulations were only dealing with circular (or spherical in 3D) particles due obviously to computational efficiency, there have been a number of attempts (Azema et al. 2007, Pena et al. 2007, Mollon et al. 2012, among others) incorporating more complex particle shapes. Though capable of simulating qualitatively the behaviour related to nonregular particles, these methods remain too simple to forecast accurately the quantitative behaviour of a granular material.

In addition to complex particle shapes, effective packing is another unsolved important issue. A packing method consists in generating in a given container a collection of particles with a desired number, density and orientation distribution. Gravitational deposition methods are straightforward but very time consuming and not suitable for arbitrary container shapes, while geometric methods may only be applied to circular/spherical particles.

The approach proposed in this paper combines and improves some existing approaches coupled with several algorithmic innovations, by following three main stages as described in Sections 2 to 4. Section 5 is devoted to a brief discussion on the accuracy and potential of the method based on two packing examples, and Section 6 presents an application of this method to the study of a granular flow through a hopper.

## 2. PARTICLE GENERATION

Describing the shape of a particle is not a straightforward task, and a large number of shape descriptors have been proposed in the literature. A complete review of the different approaches is summarized in Blott and Pye (2008). The present study only focuses on four different descriptors (see Fig. 1), namely the Elongation, the Roundness, the Circularity, and the Regularity defined as follows

$$Elongation = S/L \tag{1}$$

$$Roundness = \frac{\sum R_c}{n_c \cdot R_{insc}} \tag{2}$$

$$Circularity = \sqrt{\frac{R_{insc}}{R_{circ}}} \tag{3}$$

$$Regularity = \log\left(\frac{P}{P - P_{conv}}\right) \quad (4)$$

where $S$ is the smallest possible dimension of a grain (obtained by minimization with respect to an angle of rotation $\theta$, see Fig. 1a), $L$ is the grain dimension in the direction normal to the one of $\theta$, $R_{insc}$ is the radius of the largest inscribed circle in the particle (Fig. 1c), the $R_c$ terms correspond to the radii of the $n_c$ circles that approximate the particle contour (the method used here to fill a 2D particle with circles was proposed in Ferellec and McDowell (2008), and will be discussed later in the present article, see Fig. 1b), $R_{circ}$ is the smallest circumscribed circle of the particle (see Fig. 1c), $P$ is the perimeter and $P_{conv}$ is the convex perimeter of the particle (Fig. 1d).

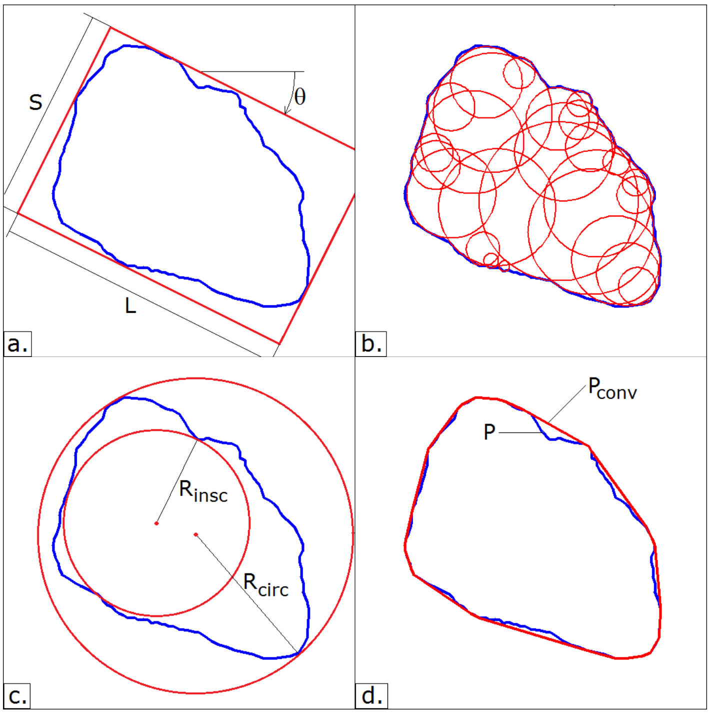


Fig. 1. Global shape descriptors of an illustrative particle: a. Elongation=0.663 and θ=–29.7°; b. Roundness=0.370; c. Circularity=0.746; d. Regularity=1.431

Besides these shape descriptors, an alternative approach proposed by Meloy (1977) has been used extensively later by Garboczi (2002) and Das (2007) among others. This approach is based on the Discrete Fourier Transform (DFT) of the contour of the grain. In 2D, the method consists in choosing a suitable centre O for the particle, and to discretize its contour in a number $N_P$ of points $P_i$ separated by a constant angle $\theta_P$ with respect to O (i.e. such that $\theta_p = 2\pi / N_p$). Thus, each point $P_i$ is defined by an angle $\theta_i$ and by a radial distance $r_i$=O$P_i$. Following the Fourier theory, the discrete signal $r_i(\theta_i)$ can be represented by the following series:

$$r_i(\theta_i) = r_0 + \sum_{n=1}^{N} [A_n \cos(n\theta) + B_n \sin(n\theta)] \quad (5)$$

where $n$ is the harmonic number and $N$ is the total number of harmonics. A DFT can be applied to the discrete signal $r_i(\theta_i)$, and will provide the discrete Fourier spectrum $\{A_n, B_n\}$ of this signal, such that:

$$A_n = \frac{1}{N} \sum_{i=1}^{N} [r_i \cos(i \cdot \theta_i)] \quad (6)$$

$$B_n = \frac{1}{N} \sum_{i=1}^{N} [r_i \sin(i \cdot \theta_i)] \quad (7)$$

The average radius of the particle $r_0$ is given by:

$$r_0 = \frac{1}{N} \sum_{i=1}^{N} [r_i] \quad (8)$$

Thus, the number $N$ of harmonics is equal to the number of points used to discretize the particle contour. It was shown in Das (2007) that the normalized amplitude of the spectrum obtained by DFT was a relevant signature for a given population of granular particles with common shape properties. This normalized amplitude is given for each harmonic $n$ by:

$$D_n = \frac{\sqrt{A_n^2 + B_n^2}}{r_0} \quad (9)$$

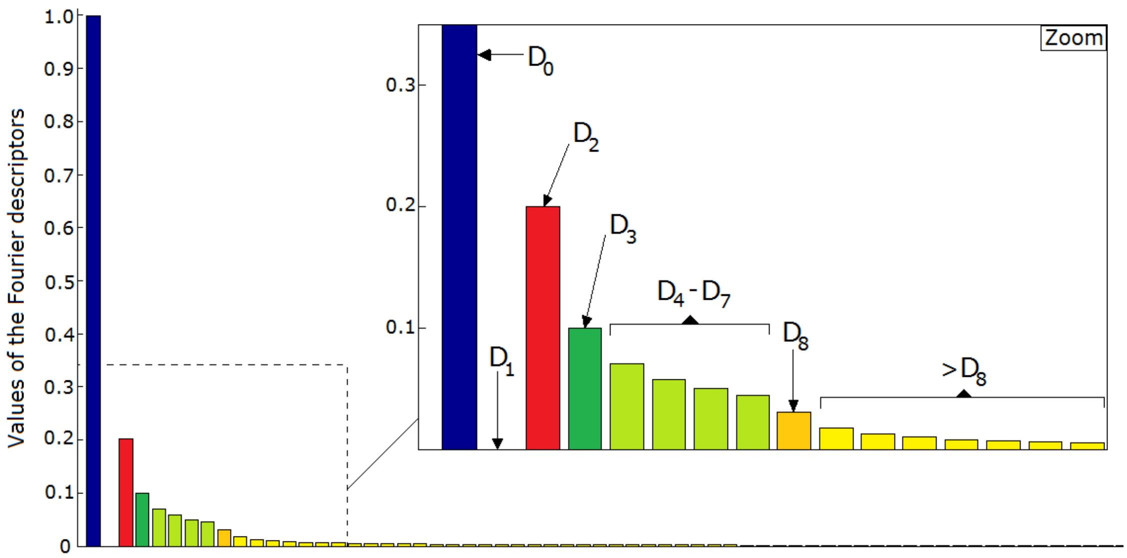


Fig. 2. Illustrative normalized amplitude spectrum

The amplitudes {$D_n$} are called "Fourier descriptors". A typical normalized amplitude spectrum is provided in Fig. 2. The first Fourier descriptor $D_0$ is equal to 1 because of the normalization, since $\sqrt{A_n^2 + B_n^2} = r_0$. $D_1$ corresponds to a "shift" of the grain contour with respect to the position of point O, and can be set to zero if this point O is well chosen. It is thus not very relevant for the shape description. On the contrary, $D_2$ is extremely important, since it describes the elongation of the particle. As proposed in Das (2007), it can be considered that the descriptors $D_3$ to $D_8$ define the main irregularities of the particle contour, and that the modes $D_n$ for $n$>8 are good descriptors of the roughness of the particle surface. For natural sands, for example, it was shown in Das (2007) that these modes decrease linearly with the descriptor number in a log-log frame. The surface roughness of a given sand can thus be described by only a slope and an intercept. In order to simplify the present analysis, simple spectra will be defined hereafter using only the values of $D_2$, $D_3$, and $D_8$. The remaining descriptors will be assumed to follow the expressions:

$$D_n = 2^{\alpha \cdot \log_2(n/3) + \log_2(D_3)} \quad \text{for } 3 < \text{n} < 8 \tag{10}$$

$$D_n = 2^{\beta \cdot \log_2(n/8) + \log_2(D_8)} \quad \text{for n} > 8 \tag{11}$$

Eq. (11) is analogous to the observations of Das (2007), i.e. the amplitudes of the modes larger than 8 decrease linearly with n in a $\log_2$-$\log_2$ frame, with a slope $\beta$. Eq. (10) is a similar expression for the modes 4 to 7, except that the slope is equal to $\alpha$. In the present study, we arbitrarily state:

$$\alpha = \beta = -2 \tag{12}$$

The Fourier descriptors are a relevant way to characterize the shape of a particle or of a population of particles, but they also may be used to perform the reverse operation, i.e. to generate a particle with prescribed features. Generation of a relevant and realistic population of particles with different shapes but with the same amplitude spectrum may be done by considering the phase angle $\delta_n$ of each mode of amplitude $D_n$. For a given particle, these phase angles are defined by:

$$\delta_n = \tan^{-1}\left(\frac{B_n}{A_n}\right) \tag{13}$$

Thus, a random particle with a prescribed amplitude spectrum {$D_n$} can be generated by randomly assigning a phase angle $\delta_n$ to each mode of order >0. Each of these random angles follows a uniform distribution on the interval [-π;π], and the discretized contour of the corresponding particle is obtained using Eq. (5), with:

$$A_n = D_n \cdot \cos\delta_n \tag{14}$$

$$B_n = D_n \cdot \sin \delta_n \tag{15}$$

This generation method is applied in the present study. Two examples of grain generations are proposed in Fig. 3, each of them following the amplitude spectrum provided in Fig. 2. It clearly appears on the figure that the random phase angles lead to different $r_i(\theta_i)$ signals and to different grain shapes, but with common visual features which can be easily recognized.

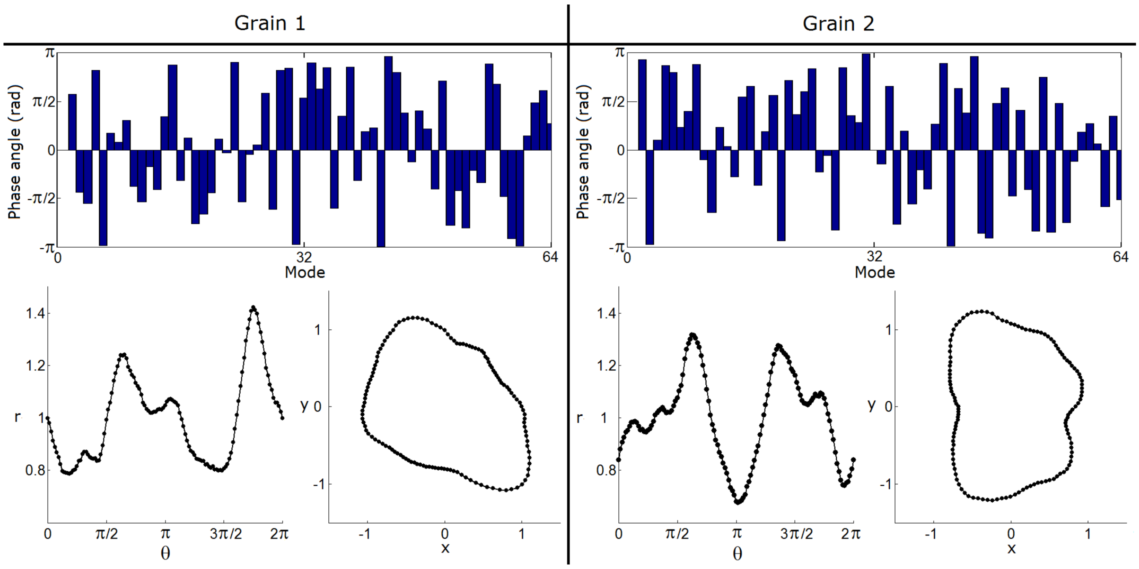


Fig. 3. Example of random generation of two grains with the illustrative spectrum in Fig. 2: random sampling of the phase angles, computation of the random signals $r(\theta)$, plotting of the corresponding particles contours.

## 3. CONSTRAINED VORONOI TESSELLATION

Before being introduced in a DEM code to simulate a given system, the generated particles have to be packed in a realistic way. A classical way to divide a domain of space in several sub-domains is to use the so-called Voronoi Tessellation (Fortune 1987), which makes use of an initial set of seeding points. It is proposed in the present study to use such a domain partition in order to pack an assembly of particles in a container, in such a way that each generated particle belongs to only one Voronoi cell. However, there is no direct method to generate directly a cloud of seeding points in such a way that their Voronoi cells follow prescribed statistical distributions in terms of sizes and orientations. A method called Inverse Monte-Carlo (IMC) was proposed in Gross and Li (2002) and Xu and Li (2009) to address this issue. The principle of this stochastic iterative method is to introduce randomly some modifications in a set of points and to accept these modifications if the statistics of the corresponding Voronoi tessellation are improved when compared to some target distributions. Thus, the set of points tends little by little to the desired distributions. The main stages of the method as proposed initially in Gross and Li (2002) are:

A. Generate an initial set of points within the selected domain, and perform a Voronoi tessellation.

B. Evaluate the statistics of this Voronoi tessellation (note that we are here focusing on the cells sizes and orientations, but it could be any other property, such as the number of neighbours or the perimeter).

C. Compute an error corresponding to the discrepancy between the current and the target statistics.

D. Move randomly one of the points of the set to another position in the domain. Compute the new Voronoi tessellation, and the new error value.

E. If the error has been reduced with respect to the previous state, accept the modification. Otherwise, ignore it.

F. Cycle on the steps D and E until the error is smaller than a prescribed threshold.

This algorithm is very robust, but has the drawback of being very slow if dealing with a large sample, because it requires the computation of the whole Voronoi tessellation at each cycle. We therefore proposed an improvement of the algorithm (Mollon and Zhao 2012). It is simply a modification of the stage D of the initial IMC algorithm. This stage is replaced by a set of operations, which consist in only modifying the local cells around the moving point. This new algorithm is not straightforward to implement but has the advantage to increase dramatically the computation speed, especially in the case of large samples. Thanks to this modification, the computation time of each cycle of IMC is independent from the total number of points.

## 4. CELL FILLING

The IMC methodology presented in the previous section makes it possible to build up a partition of a container-domain in a number of polygonal sub-domains with prescribed statistics in terms of size and orientations. In order to model accurately the packing of a granular assembly, each of these cells may be filled with a particle generated using the method presented in Section 2. However, to take advantage of the prescribed properties of the Voronoi tessellation obtained by IMC, the particles should be able to reproduce the properties (size and orientation) of the cells in which they are generated. A method to respect this condition when filling a polygonal cell with a particle with a given Fourier spectrum is proposed in this section. The principle of this method is to perform for each particle an optimization such that this particle should occupy a prescribed proportion of the surface of the polygonal cell, and that it should be entirely contained inside the cell. This optimization is performed for seven variables : the phase angles of the modes $D_2$ to $D_7$ (i.e. the modes that are considered as controlling the particle shape, as proposed in Section 2), and the average radius $r_0$ of the particle. The particle shape is obtained from the following minimization, using the notations of Fig. 4:

$$\min_{r_0,\delta_2,\delta_3,\delta_4,\delta_5,\delta_6,\delta_7}\left(\frac{S_p}{S}-F_S\right)^2 \quad \text{subjected to} \quad r_i < r_{\max,i}\,\forall\,\theta_i \tag{16}$$

where $F_s$ is the target solid fraction of the particle in the cell (i.e. the proportion of the surface of the cell covered by the particle), $S_p$ is the particle surface, $S$ is the cell surface, and $r_i$ and $r_{max,i}$ are the radial distances from the centre to the edges of the particle and of the cell respectively, for an angle $\theta_i$ with $1 \le i \le 128$ (if the particle contour is discretized by 128 points). The set of variables $(r_0, \delta_2, \delta_3, \delta_4, \delta_5, \delta_6, \delta_7)$ obtained from this optimization is combined with the chosen discrete normalized amplitude spectrum $\{D_n\}$ and with random values for the remaining phase angles ($\delta_n$ for $n$>7), and the final contour of the particle is computed from Eqs. (14), (15), and (5). More details about the cell-filling algorithm and the links between the shape descriptors and the Fourier descriptors may be found in Mollon and Zhao (2012).

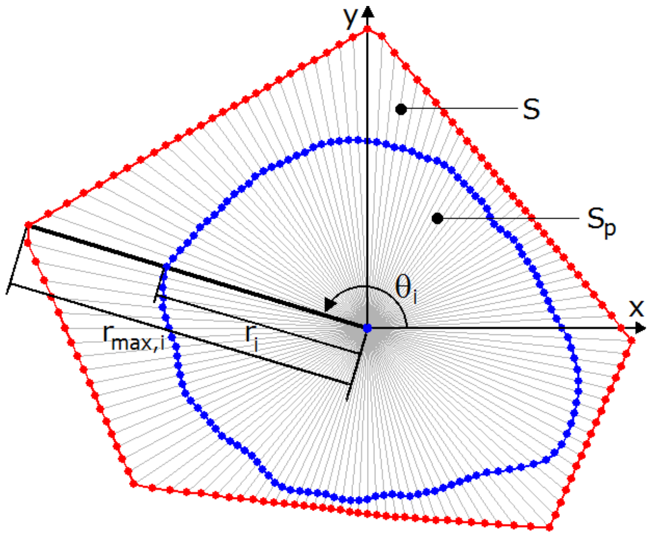


Fig. 4. Notations used in the cell-filling method

The particle shape defined by this optimization method cannot be introduced directly in a DEM code because usual codes are not able to perform neighbourhood and contact detections with arbitrary shapes. One of the most convenient methods to deal with this issue is to use the Overlapping Discrete Element Clusters (ODEC) framework, as proposed in Ferellec and McDowell (2008). In this framework, the complex shape of the particle is filled with a collection of overlapping disks (spheres in 3D) which are rigidly assembled as a single "cluster". Such a cluster may then be introduced in a DEM code (able to handle neighbourhood and contact detections of discs or spheres), in such a way that no internal effort develops between the "slave elements" of a given cluster. This method is used in the remainder of this article, and the interested reader may find a detailed description of the ODEC algorithm in Ferellec and McDowell (2008).

## 5. PACKING EXAMPLES

To illustrate the potential of the method, two packings are performed and detailed hereafter. They make use of the illustrative Voronoi tessellations described earlier in this article. These rather dense packings are composed of 500 particles each, and their main features are:

- Example 1: large size dispersion, isotropic orientations, moderate Elongation, low Roundness and Regularity.

- Example 2: small size dispersion, mostly horizontal orientation, elongated particles with high Roundness and Regularity.

The properties of size dispersion and of orientation are directly obtained from the characteristics of the Voronoi tessellations as described in Section 3, while the properties related to the shape descriptors are obtained by choosing carefully the discrete Fourier spectrum. The target solid fraction is set to 0.65 in both examples. The Fourier descriptors and resulting solid fractions are provided in Fig. 5, as well as the obtained packings. More precisely, for each of the two examples, Fig. 5 provides a detailed view of the packing, two plots of the packing for which the colours of the particles correspond respectively to sizes and orientations, the target and obtained size distributions, the target and obtained rose diagrams of the particles orientations, and the expected average values and obtained distributions of the four shape descriptors (Elongation, Roundness, Circularity and Regularity). All these results show that a fairly good match is obtained between the target and resulting statistics of the packings. The plots of the two packings illustrate the potential of the method and its ability to generate a wide range of granular materials in very diverse configurations.

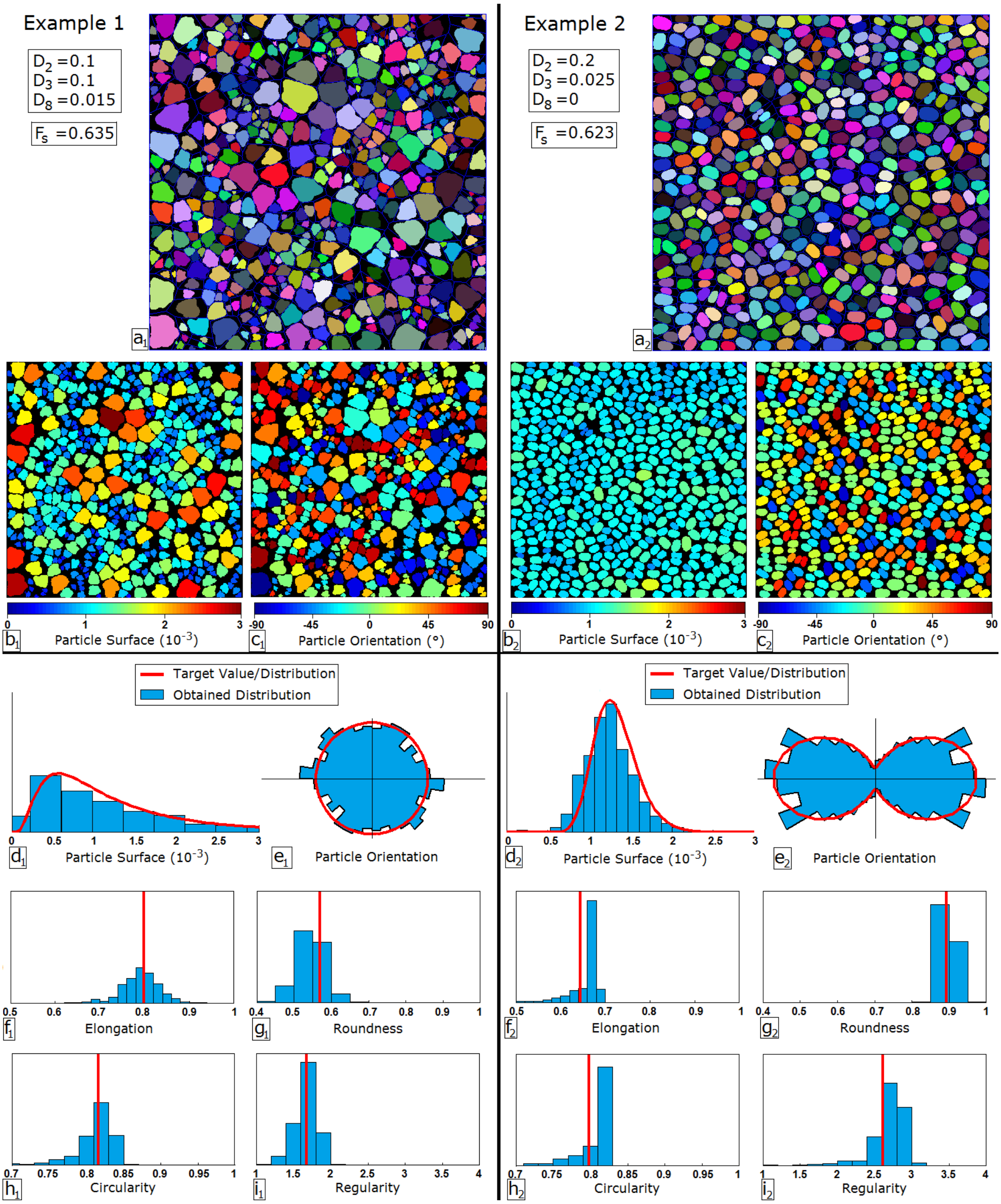


Fig. 5. Two detailed examples of packing: ($a_1$, $a_2$) Detailed view of the packing; ($b_1$, $b_2$) Particle sizes; ($c_1$, $c_2$) Particle orientations; ($d_1$, $d_2$) Target and obtained size distributions; ($e_1$, $e_2$) Rose diagram of the target and obtained orientation distributions; ($f_1$, $f_2$) Target value and obtained distribution of Elongation; ($g_1$, $g_2$) Target value and obtained distribution of Roundness; ($h_1$, $h_2$) Target value and obtained distribution of Circularity; ($i_1$, $i_2$) Target value and obtained distribution of Regularity

## 6. APPLICATION TO A GRANULAR FLOW THROUGH A HOPPER

In this section, a simple demonstrative example is shown by employing the aforementioned approaches to reproduce some experimental results obtained by Nakashima et al. (2011). Nakashima et al. (2011) have conducted their experiments by flowing Toyoura sand through a hopper under different gravity conditions (though we are only focusing here on the results obtained under 1G).

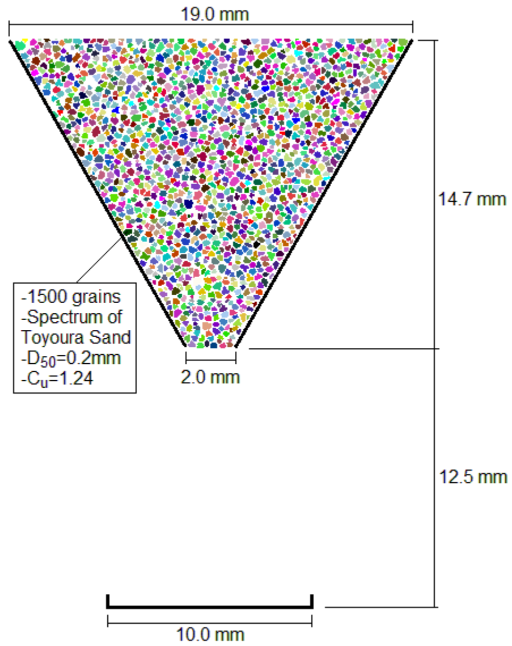


Fig. 6. Layout of the simulation

The Fourier spectrum of Toyoura sand is obtained from Das (2007), and the true size distribution ($D_{50}$=0.2mm, $C_u$=1.24) of this sand is used to replicate the experiments. However, in order to limit the computational cost, the scale of the experimental apparatus is reduced by a factor 10, leading to the final dimensions shown in Fig. 6. Moreover, the experiment is simplified to a 2D framework wherein the packing method described in the previous sections is used to generate the sand sample (1500 particles, each composed of approximately 20 overlapping discs). The obtained granular system is introduced in the commercial software Itasca PFC2D to simulate the hopper flow. In the simulation, the following mechanical parameters are adopted:

Table 1. Mechanical parameters of the PFC2D simulation

| | |
|---|---|
| Local damping coefficient | 0.7 |
| Contact normal and tangential stiffness | $10^5$ |
| Contact friction coefficient | 0.05 |

The simulated flow and deposition processes of the sand sample are plotted in Fig. 7 (colours corresponding to the velocities of the grain). It appears in this figure that the velocity field in the hopper and during the deposition is not symmetric and not continuous. This flow complexity, likely to be related to the non-circularity of the particles, will be the topic of future studies. Fig. 8 shows a detailed view of the sand deposit. A post-processing algorithm similar to the one described in Mollon et al. (2012) is used to determine a close envelope of the deposit, as shown in white solid line in the figure. Such an envelope may be useful, for example to assess the global void ratio of the deposit.

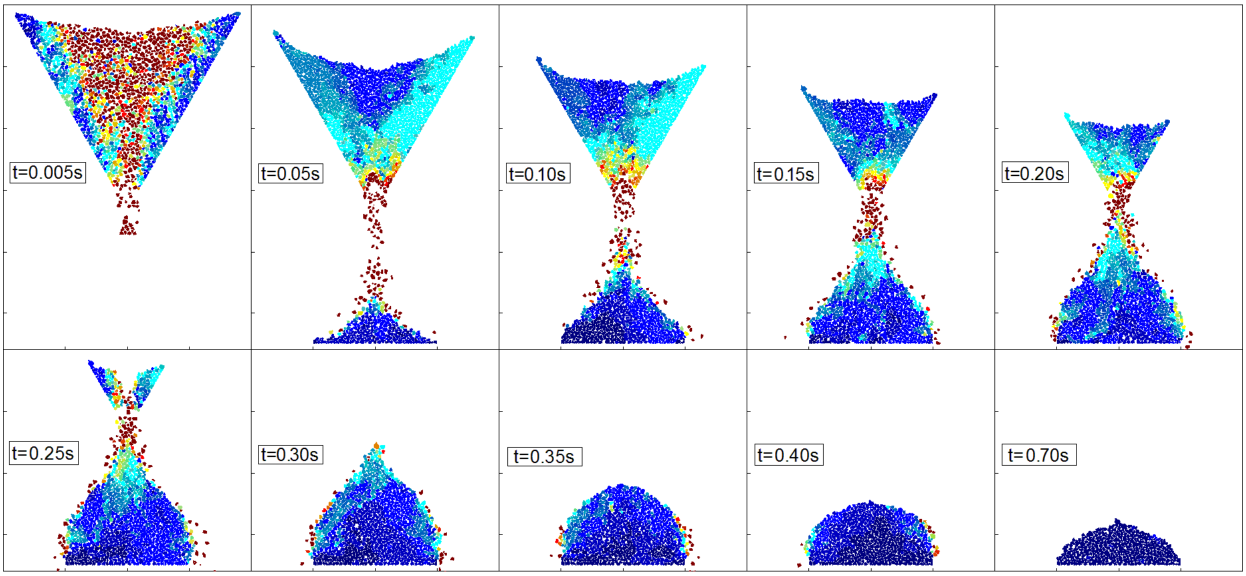


Fig. 7. Granular flow through the hopper and deposition (colour indicates velocity)

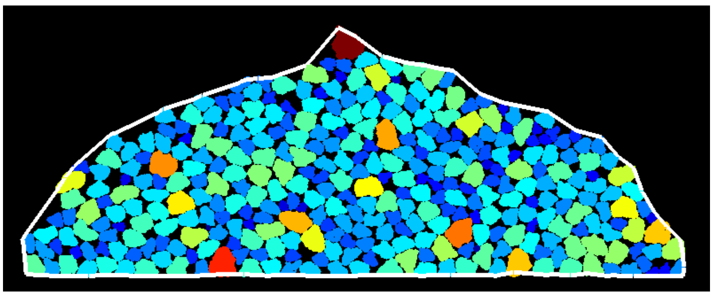

Fig. 8. Geometry and contour of the final deposit

A sensitivity study is performed on the three mechanical parameters (local damping, contact stiffness, and contact friction) to evaluate their relative influence on the shape of the deposit. The results are plotted in Fig. 9. As is shown, both the contact stiffness and the contact friction have a significant influence on the repose angle, while the local damping does not. It also appears that the small number of particles used here is not sufficient to achieve a realistic triangular shape for the deposit, and that it is therefore very difficult to obtain a reliable value of the numerical repose angle. However, a comparison with the expected deposit shape (plotted in Fig. 9 using the repose angle obtained experimentally in Nakashima et al. 2011) shows that this simulation is able to reproduce some satisfying deposition behaviours using very low values of the contact friction coefficient (between 0 and 0.1). For comparison, it is reported in Nakashima et al. (2011) that a contact friction coefficient of 0.6 coupled with a coefficient of rolling friction of $1.6*10^{-5}$ was required to reproduce the experimental results with a discrete modelling based on disc-elements. The use of complex-shaped elements thus allows a realistic modelling of sands without using the coefficient of rolling friction, which is a parameter quite difficult to calibrate.

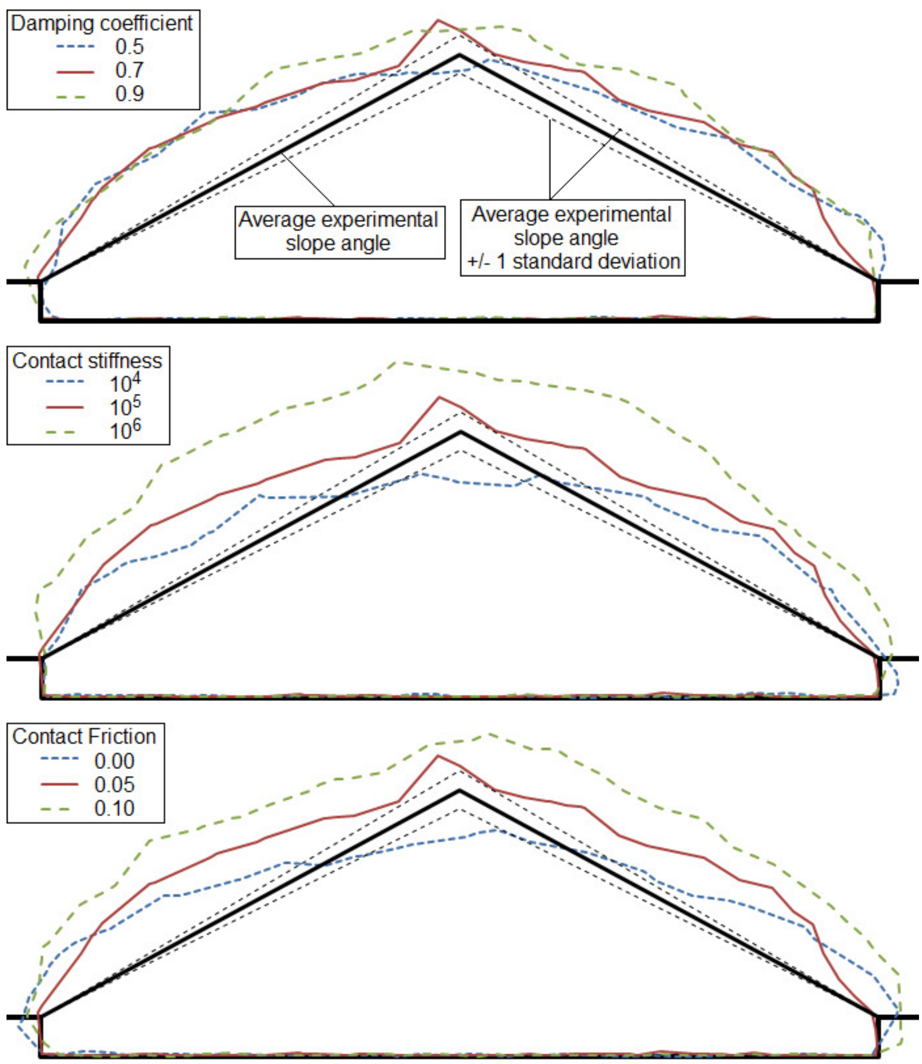


Fig. 9. Sensitivity study on the mechanical parameters of the simulation (Damping coefficient, contact stiffness, and contact friction coefficient)

## CONCLUSION

This article presents a new method for the generation and packing of samples of granular materials for introduction in a DEM code. Compared to existing methods, this new framework has the advantage to be able to deal with complex particle shapes and anisotropic particle orientations, in any container geometry. The proposed method is based on several existing approaches developed in different frameworks as well as on several algorithmic innovations. Its main principles are (i) to generate a Constrained Voronoi Tessellation of the container in a large number of polygonal subdomains respecting some target statistics in terms of sizes and orientations, and (ii) to fill each of these subdomains with a virtual particle respecting some target shape characteristics. To achieve the first of these goals, an existing stochastic and iterative method called Inverse Monte-Carlo (IMC) method was chosen, improved, implemented and fully tested. The second purpose of the study was fulfilled by using a new method of random particle generation based on the Fourier Descriptors approach, and by developing an original algorithm to fill efficiently each Voronoi cell with such a generated particle. As shown in the two examples developed in the article, the proposed packing methodology makes it possible to generate a wide range of granular samples, with very different characteristics in terms of container shape, particle number, size distribution, particles orientations, elongations, shapes, and packing density. In the framework of computational geomechanics, the experimental data already available in scientific literature (such as the Fourier amplitude spectra provided in Das (2007) for several sands) make it possible to apply this method directly to the modelling of real materials. A short example of application is provided in the last section of this article, which describes the simulation of sand flow through a hopper and deposition. This example emphasizes the potential of the proposed packing methodology in a wide range of applications.

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