A Statistically-based Approach on Reconstructing Sand Particles for Discrete Modeling

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ABSTRACT: This paper presents an overview of a statistically-based Fourier-Voronoi approach recently proposed by the authors to generate packing of granular particles with key characteristics reproduced from real sands. The key sand properties identified in this approach include the grain size distribution, density, particle orientation and the shape characteristics. Four important shape factors are chosen to characterize the shape of a particle, including elongation, circularity, roundness and regularity. To generate a packing of particles, a 2D container of arbitrary shape is discretised by a Voronoi tessellation with prescribed cell size and orientation distributions. Each of the Voronoi cells is then filled by a particle with the prescribed shape characteristics. The proposed method is shown to be capable of realistically reproducing a variety of granular sands based on available experimental data. This method is further generalized to reproduce 3D sand shapes based on the Fourier descriptor concept, with demonstrative examples on two sands (Michigan Beach sand and Ottawa sand). The proposed methods provide a rational and systematic way to reconstruct real sand particles for discrete modelling.

KEYWORDS: Sand particle, shape, statistics, Fourier-Voronoi approach, discrete modeling

1 INTRODUCTION

Accurate modelling of the micromechanical behaviour of a granular medium needs effective characterization of its particle morphology. It is well known that the shape and surface characteristics of soil particle may significantly affect the microscopic behaviour such as inter-particle contacts, soil fabric, particle kinematics and particle crushing, as well as macroscopic behaviour including soil stiffness, shear strength, liquefaction, strain localization, dilation and critical state as well as residual soil behaviour (Santamarina & Cho, 2004). While discrete-based modelling approach, such as Discrete Element Method or Molecular Dynamics (MD), has prevailed in the research of granular media from grain level, systematic approaches of accurate characterization and reconstruction of particle shapes for discrete simulations have yet to be developed. Conventional approaches in DEM/MD have considered oversimplified discs (in 2D) or spheres in generating an assembly of particles. Thought the idealization may offer various advantages in terms of numerical manipulation and computational efficiency, it loses important information regarding the shape and surface properties of the particles that may significantly affect the material behaviour. To model non-circular/non-spherical particles, different approximation approaches have been proposed, including the use of ellipses/ellipsoids, polygons/polyhedrons and forming of cluster by merging multiple circular/spherical particles together (see, e.g., the ODEC [overlapping Discrete Element Cluster] method proposed by Ashmawy et al., 2003 and Sallam, 2004 for the 2D case; the ellipsoid method by Lin & Ng, 1997; the polyhedron-based method by Ghaboussi & Barbosa, 1990; ODEC in 3D by Das, 2007 and among others).

This paper presents an overview of a method recently proposed by the authors for reconstructing real sand particles and generating granular assemblies for DEM study, based on statistical characterization of particle shapes and other important information obtained from experiments (Mollon & Zhao, 2012, 2013). In addition to important factors such as the grain size distribution, density and particle orientation, we consider the shape characteristics of sand grains by defining four shape descriptors, including elongation, circularity, roundness and regularity which can be calibrated from experimental observation of sand particles. Voronoi tessellation is then employed to generate particle packing constrained by these key factors of sand. The Fourier-Voronoi approach is first demonstrated by reconstruction of 2D sand grains, and is then extended to the general 3D case with the aid of a specially developed revolving-stretching-morphing technique. The accuracy and robustness of the proposed method are demonstrated by several examples. Usefulness of the method for future DEM study of granular soil is discussed.

2 FOURIER SHAPE DESCRIPTORS FOR REALISTIC SAND PARTICLE RECONSTRUCTION

Four descriptors of particle shape, namely the elongation, the roundness, the circularity and the regularity, are chosen to characterize the shape of granular sand. Figure 1 illustrates the definitions of the four descriptors. A discrete form of shape descriptors proves to be practically more useful. To this end, the Discrete Fourier Transform (DFT) is employed to discretise the surface of a grain (Ehrlich and Weinberg, 1970) (practically a Fast Fourier Transformation is commonly used).

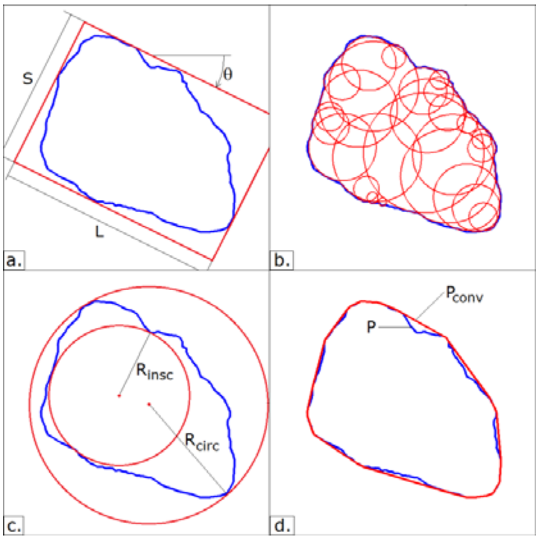

Figure 1. Illustrations of shape descriptors for a granular particle in 2D (from Mollon & Zhao, 2012). (a) Elongation = S/L; (b) Roundness = $\sum R_c / (n_c \cdot R_{insc})$ (R_c denotes the radius of circles approximating the corners of the particle contour, and n_c is its total number); (c) Circularity = $\sqrt{R_{insc}/R_{circ}}$; (d) Regularity = $\log\left[P/\left(P-P_{conv}\right)\right]$ (P is the perimeter and P_{conv} is the convex perimeter of the considered particle).

In the 2D case, the surface contour of a grain can be discretised by a number of points. With a chosen centre, the radial distance of each contour point to the centre can be expressed as follows:

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

where n is the harmonic number and N is the total number of harmonics. Application of DFT to Eq. (1) leads to its discrete Fourier spectrum, with its real and imaginary parts respectively given by:

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

$$B_n = \frac{1}{N}\sum_{i=1}^{N}\left[r_i \sin(i \cdot \theta_i)\right] \qquad (2)$$

and the following average radius for the particle

$$r_0 = \frac{1}{N}\sum_{i=1}^{N}\left[r_i\right] \qquad (3)$$

As a relevant signature for a given particle system with common shape characteristics, the normalized amplitude of the spectrum obtain above by DFT is taken to describe the particle shape:

$$D_n = \frac{\sqrt{A_n^2 + B_n^2}}{r_0} \qquad (4)$$

Amongst all the normalized amplitudes $\{D_n\}$, $D_3 = 1$; $D_1 = 0$; D_2 describes the elongation of the particle; D_3 to D_8 define the major irregularities of the particle contour. For the rest, D_n ($n > 8$) are related to the roughness of the particle surface which decrease linearly with the descriptor number in a log-log scale. Mollon & Zhao (2012) adopted three of the Fourier descriptors, D_2, D_3 and D_8, together with the following interpolation functions for other descriptors to characterize the shape of particle

$$\begin{cases} D_n = 2^{\alpha \cdot \log_2(n/3) + \log_2(D_3)} & \text{for } 3 < n < 8 \\ D_n = 2^{\beta \cdot \log_2(n/8) + \log_2(D_8)} & \text{for } n > 8 \end{cases} \qquad (5)$$

By adopting $\alpha = \beta = -2$, the influence of the three Fourier descriptors on the shape of a randomly generated particle is demonstrated in Figure. 2.

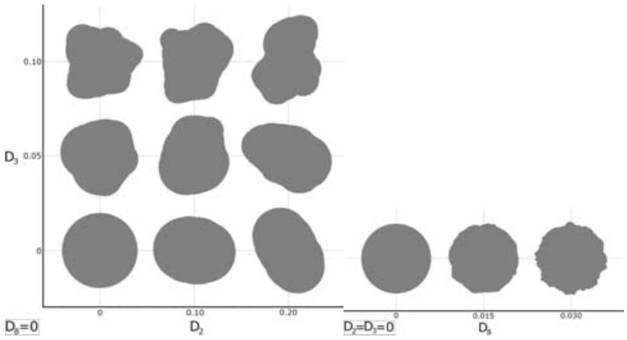

Figure 2 Influence of Fourier descriptors D_2, D_3 and D_8 on the shape of randomly generated particle (from Mollon & Zhao, 2012).

3 CONSTRAINED FOURIER-VORONOI METHOD

3.1 *2D Sand Packing Generation*

In conjunction with the above Fourier shape descriptors, Mollon & Zhao (2012) proposed a constrained Voronoi tessellation method to generate 2D sand packing with realistic particle shape and other preferences such as relative orientation and grain size distribution (GSD). The principle is as follows. A domain under consideration is partitioned first by Voronoi tessellation cells. An inverse Monte-Carlo (IMC) method is then employed to evaluate the statistics of the Voronoi cells and compare them with the targeted one imposed by such constraints as the preferred particle shape, GSD and preferred orientation. The Voronoi cells are then revised iteratively to reduce the error between the two statistical quantities. The algorithm has been found robust and efficient enough for general cases. Based on the IMC-generated Voronoi cells, an ODEC method is then applied to fill each cell with a particle of desired shape and other constraints. Figure 3 gives two illustrative examples of packings with different targeted features.

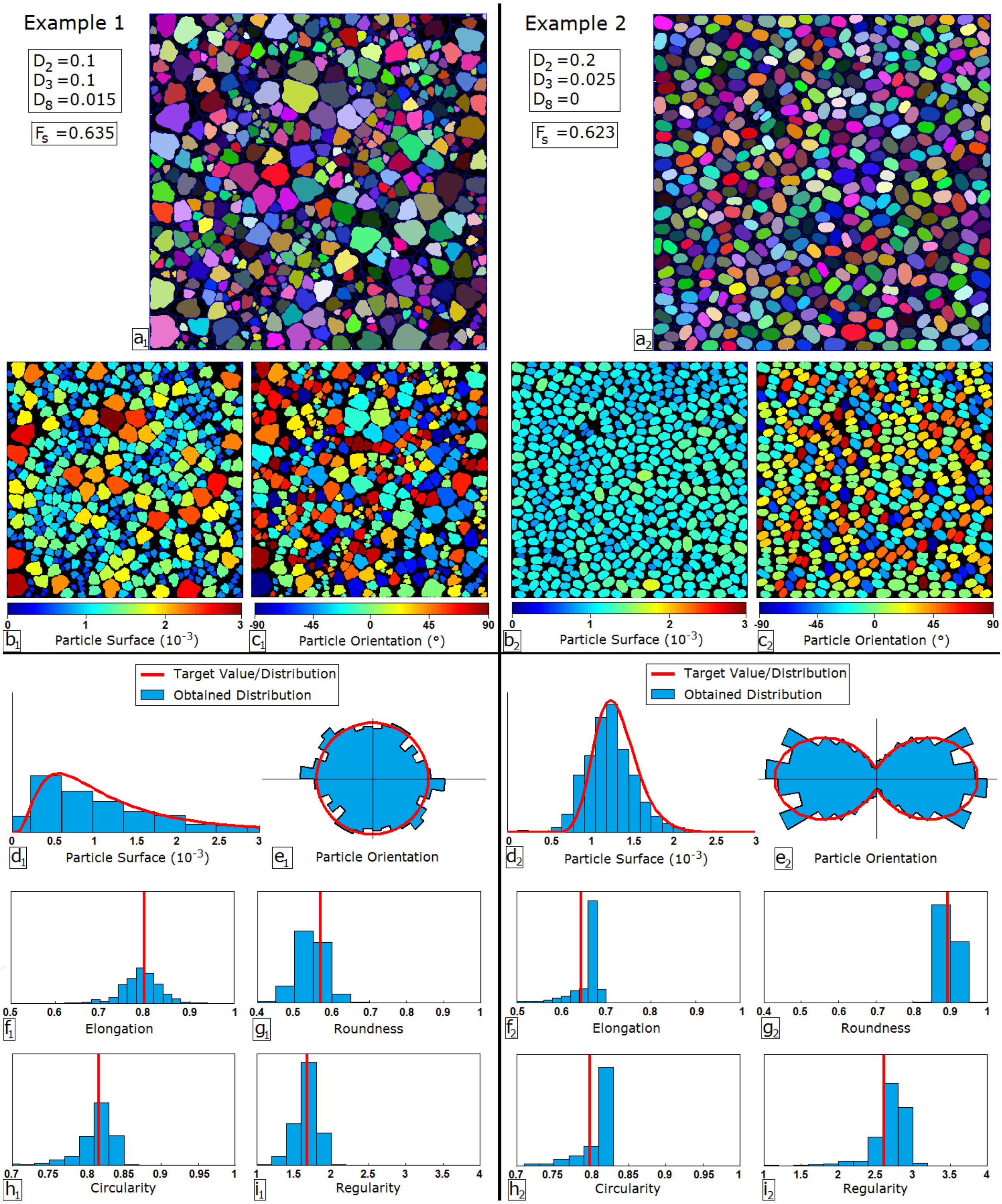

Figure 3. Two illustrative examples of sand packing generated by the constrained Fourier-Voronoi approach (from Mollon & Zhao, 2012)

3.2 *Extension to 3D Particle Reconstruction*

The proposed Fourier-Voronoi approach has more recently been extended to 3D reconstruction of sand particles (Mollon & Zhao, 2013). Essentially, the extension considers the profiles of three orthogonal cross sections for a real sand particle. Each of them is generated by the constrained Fourier-Voronoi method entailed above to reconstruct a 2D profile of the particle. The four vertical half-profiles are then revolved around their respective axis. A stretching and morphing scheme is then applied to merge the four revolved bodies together to form a 3D particle surface. Figure 4 demonstrates the procedure of revolving of the orthogonal contours, stretching and morphing them to form a 3D particle surface. Fig. 5 further employs two examples of real sand, one being the Michigan Beach sand and the other the Ottawa sand (reported by Vardhanabhuti, 2006), wherein good performance of the proposed method for 3D particle reconstruction is evident.

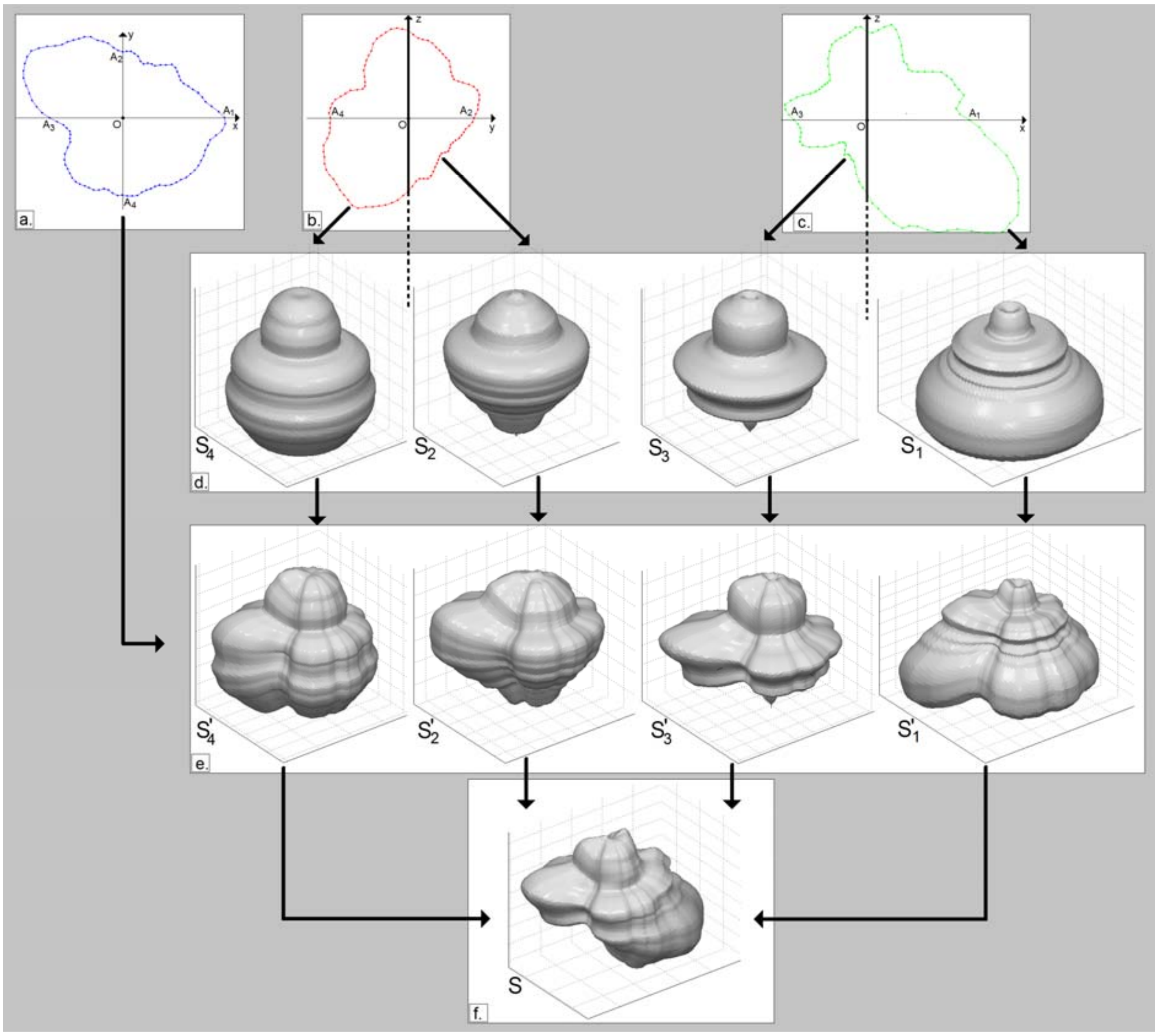

Figure 4. Illustrative procedure of reconstructing 3D surface for a sand particle based on the constrained Fourier-Voronoi approach (from Mollon & Zhao, 2013).

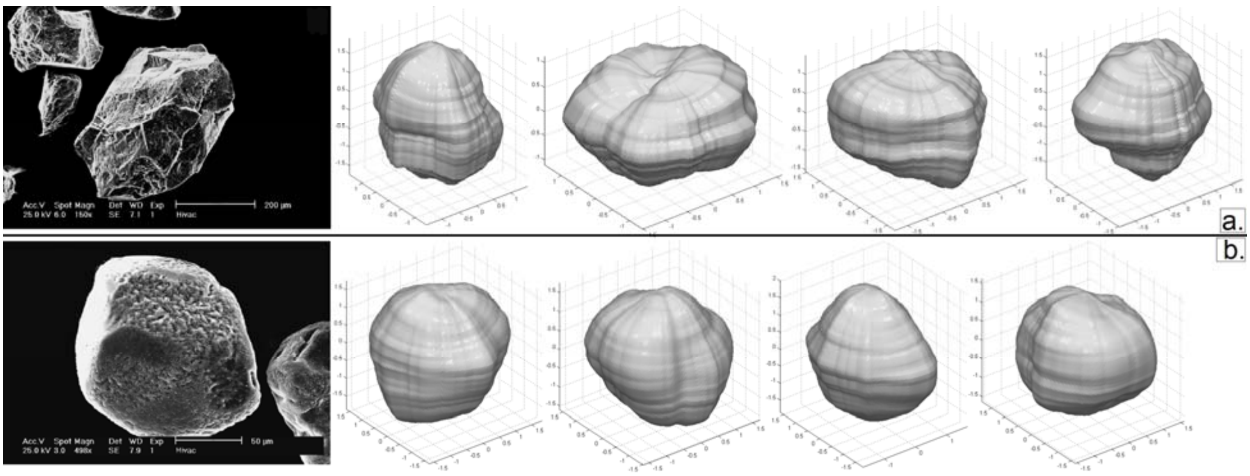

Figure 5. SEM grain pictures (from Vardhanabhuti, 2006) of (a) Michigan Beach sand and (b) Ottawa sand, and the virtual 3D grains reconstructed with their Fourier spectra (viewed from different angles) (from Mollon & Zhao, 2013).

4 CONCLUSION

This paper summarised a statistically-based Fourier-Voronoi approach recently proposed by the authors (Mollon & Zhao, 2012, 2013) on generating realistic particles with their key characteristics reproduced from real sands for discrete modelling of granular media. Key to the methodology is the selection of proper Fourier shape descriptors and their use in a constrained Fourier-Voronoi approach. Based on a revolving-stretching-morphing scheme, the proposed Fourier-Voronoi approach was further generalized to reconstruct 3D sand particles. The capacity and performance of the proposed methods were demonstrated by several examples on real sands. The study paves a way for systematic reconstruction of sand particles based on experimental data for use in discrete modelling of granular media.

5 ACKNOWLEDGEMENTS

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