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# 3D generation of realistic granular samples based on random fields theory and Fourier shape descriptors

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**Abstract**

The inability of simulating the grain shapes of granular media accurately has been an outstanding issue preventing particle-based methods such as discrete element method from providing meaningful information for relevant scientific and engineering applications. In this study we propose a novel statistical method to generate virtual 3D particles with realistically complex yet controllable shapes and further pack them effectively for use in discrete-element modelling of granular materials. We combine the theory of random fields for spherical topology with a Fourier-shape-descriptor based method for the particle generation, and develop rigorous solutions to resolve the mathematical difficulties arising from the linking of the two. The generated particles are then packed within a prescribed container by a cell-filling algorithm based on Constrained Voronoi Tessellation. We employ two examples to demonstrate the excellent control and flexibility that the proposed method can offer in reproducing such key characteristics as shape descriptors (aspect ratio, roundness, sphericity, presence of facets, etc.), size distribution and solid fraction. The study provides a general and robust framework on effective characterization and packing of granular particles with complex shapes for discrete modelling of granular media.


*Keywords:* Granular media; Discrete modelling; Particle shape generation; Particle packing; Random fields; Constrained Voronoi tessellation

## 1. Introduction

Granular materials are of primary interest for a wide range of industrial applications, including civil and chemical engineering, powders and pharmaceutical industries, mining and energy industries. They are meanwhile topics of interest for researchers across communities of granular physics, geophysics, tribology, nanoparticles and colloïds sciences. In the simulation and analysis of granular media, Discrete Element Method (DEM) has become a standard computational tool now. Early DEM studies on granular materials have considered circular or spherical particles due primarily to the simplicity and convenience in terms of contacts detection and repulsive forces computation [1].

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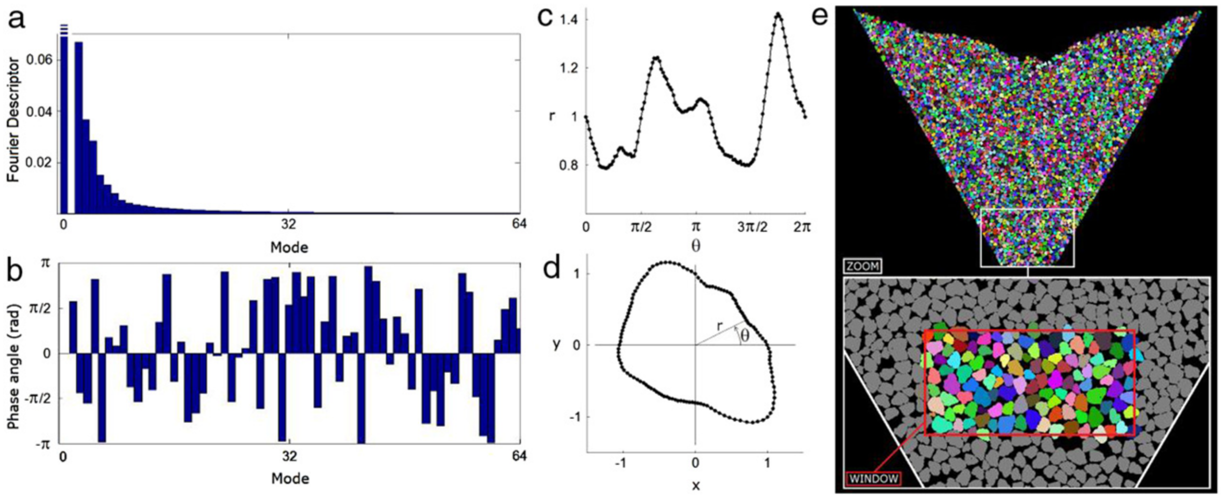


Fig. 1. Existing method for 2D generation of random particles [10,4]: a. Input Fourier spectrum; b. Random phase angles; c. Random signal; d. Same signal expressed in a polar frame; e. Application to the simulation of a 2D hopper flow.

It has become increasingly clear that these oversimplifications of particle shape in DEM modelling cannot provide adequately accurate and quantitative predictions on the behaviour of granular materials, and improved consideration of the realistic shape of granular particles has become a current trend. To this end, various non-circular shapes have been proposed to approximate the real shape of particles, ranging from clusters of discs or spheres (e.g. [2–9]), polygons, ellipses [10] and polyarcs to super-ellipsoids [11–13], cylinders [14] and polyhedrons or sphero-polyhedrons [15–22]. Though they have helped to gain various improvements on the understanding of granular behaviour, these approaches remain to be too simplified approximations to provide accurate description of the real shape of particles. Due to these geometric simplifications, various assumptions with obscure physical meanings have to be made on contact parameters (such as friction, stiffness, viscosity) in DEM simulations and need to be calibrated by back analysis, which brings in more or less phenomenological ingredients into DEM. The DEM simulations based on these simplified considerations remain a long way from providing quantitative predictions on the real behaviour of granular materials. There is a need for systematic approaches to be developed to effectively represent the realistic geometric characteristics of granular particles before incorporation in DEM modelling.

In this study, we aim to develop a novel statistical approach to solve the above issues. In particular, we identify statistical properties representing the unique shape characteristics of a granular material to provide faithful reference for generating realistic three-dimensional packing of particles for DEM modelling. The study is based on an early two dimension work by the authors [23] wherein the concept of Fourier descriptors was employed. Fourier shape descriptors were first introduced in [24] for particle shape characterization and were further applied by several authors to sand characterization (see, e.g. [25]). It was shown that the average normalized Fourier spectrum (Fig. 1a) of the 2D projected contours (expressed in polar coordinates) of a family of particles may embody a relevant signature of the shape features of these particles. The amplitude of Mode $D_2$ of such a spectrum is a good descriptor of the particle elongation, the next few modes contain information on the main shape irregularities, and the high-frequency modes describe the surface roughness of the particle. The normalized spectrum of a population of granular particles is rather easy to obtain experimentally, using, for example, micro-photographs coupled with simple image treatment algorithms and discrete Fourier transform [25]. A particular innovation in [23] was to reverse the concept, by using such a spectrum as the starting point for generating random particles with prescribed shape features. This was done by performing an inverse Fourier transform on a chosen spectrum (Fig. 1a), with the randomness being introduced by means of random phase angles for each Fourier mode (Fig. 1b). The generated 2D particles were then packed in a chosen virtual container with a prescribed granular density based on a constrained Voronoi tessellation approach. The working program (coded in a MATLAB and available for free download at http://guilhem.mollon.free.fr) can now help us generate a packed 2D granular sample with perfectly controlled properties including size distribution, elongation, roundness, circularity, regularity, orientation anisotropy and void ratio. This program was successfully applied to the modelling of a 2D sand flow through a wedge-shaped hopper (see Fig. 1e and Refs. [4,26]).