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# 3D characterization of general-shape sand particles using microfocus X-ray computed tomography and spherical harmonic functions, and particle regeneration using multivariate random vector

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ABSTRACT

The morphological features of sand particles play a key role in the mechanical response of the particle assemblage. Advancement of microfocus X-ray computed tomography (μXCT) technology has enabled 3D visualization of particles at the grain-scale with reasonably high resolution to reveal the particle morphology. This paper utilizes the real part of spherical harmonic (SH) functions to describe the morphology of general-shape sand particles acquired from μXCT images. The influence of the maximum degree of SH functions and mesh fineness on the determination of size and shape descriptors of the particles are systematically investigated. Correlations between different shape descriptors of the studied sands are examined. Utilizing principal component analysis (PCA) and the empirical cumulative distribution function (ECDF), a probabilistic approach considering both intrinsic and phenomenological correlations between SH coefficients is proposed to three-dimensionally regenerate the sand particles. Based on comprehensive and quantitative comparisons between the morphological characteristics of scanned and generated particles, we conclude that the proposed approach performs satisfactorily.


## 1. Introduction

Sand is probably the most common natural granular powder people encounter in their daily lives. At the same time, it is a common geomaterial found in many types of engineering construction, such as slopes, structure foundations, embankments, tunnels, *etc.* [1–4]. An extensive number of studies have indicated that the macroscopic mechanical behaviors of sand, such as stiffness, shear strength and shear-induced dilatancy, are closely related to particle morphology [5–13]. Traditionally, particle morphology is commonly inferred from two-dimensional (2D) projected images obtained by scanning electron microscope (SEM), optical microscopy or laser beam systems [14–15]. Particle shape analysis is subsequently performed on these 2D images. Despite its convenience and relatively low cost, it can be anticipated that a 2D-based study cannot truly represent the three-dimensional (3D) nature and characteristics of particles. The recent development of microfocus X-ray computed tomography (μXCT) technology [16] has enabled researchers to visualize the 3D morphological features of particles through a stack of images at micrometer resolutions at a reasonable cost.

There are a number of methods to quantify the 3D shape characteristics of a particle from its μXCT images. As summarized in [17], these methods can be classified into three categories: direct computing from voxel assembly of images; evaluating from reconstructed triangular mesh surface; and calculating from the surface reconstructed by 3D spherical harmonic (SH) analysis. Although the last approach involves more complex algorithms and computational effort, it allows not only the characterization of non-convex particles and the evaluation of various shape descriptors (*e.g.*, particle aspect ratio, angularity, convexity, *etc.*) using the derived SH coefficients but also statistical regeneration of the studied particles with proper numerical procedures [18–22]. Generation of 3D particles resembling their morphological features is a crucial step to regenerate a realistic particle assemblage in the discrete element method, which has become a promising numerical tool to investigate the micro-macro linkage of the mechanical behavior of granular materials [22–23].

Spherical harmonics were originally used to analyze radial or star-shaped objects, which are defined as objects with all line segments connecting the center of the object to any point on its surface lying entirely within the object body [24]. This type of SH analysis, which involves expansion of the distance between the center of the object to a point on its surface as a function of the polar and azimuthal angles, has been successfully applied in some cases of concrete aggregates and sand particles [18–20,22]. However, many objects exhibit concave

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surfaces which do not follow the star-shaped description, *i.e.*, some lines connecting the center of object to points on the object surface lie outside the object body. Sand particles, make no exception, are not confined to star-like shapes. To reconstruct general-shape objects, Brechbühler et al. [25] proposed a method in which the three Cartesian coordinates of the object surface are represented by functions of the polar angles. The method was further developed by Shen and Makedon [26] and Shen et al. [27] to describe and reconstruct bioinformatic structures. More recently, Zhou et al. [21] adopted this approach to analyze a few Leighton Buzzard sand (LBS) and highly decomposed granite (HDG) particles, of which particle non-convexity induced by geological weathering was commonly seen. Their results showed that some basic characteristics of the natural particles, such as volume and surface area, can be well reproduced when the maximum degree of SH functions is set to approximately 10. In addition, it is worth mentioning that most of the previous studies used the full spectrum of SH functions in which the function coefficients are complex numbers [21,25–27]. However, the use of complex number not only doubles the number of numeric values that need to be determined but also brings along difficulty in interpreting coefficients owing to the introduction of phase angles. Furthermore, some important issues for the generation of general-shape virtual numerical particles by means of SH functions, including the intrinsic relationships among SH coefficients at the first degree, were not addressed previously. Failing to address these issues may lead to the generation of erroneous grains that significantly deviate from real particles.

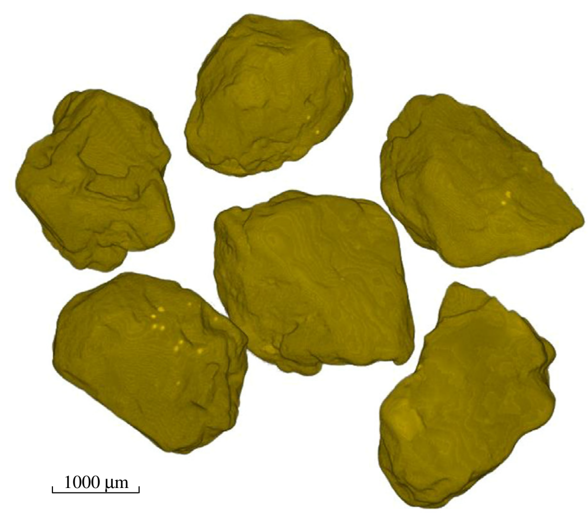
In this study, attempts have been made to use only the real part of the SH functions to describe, analyze and reconstruct the μXCT-scanned sand particles. The approach has been validated by comparing the results with those using the full spectrum SH functions. Afterwards, the influence of the maximum SH degree ($N$) and mesh fineness characterized by the numerical incremental steps of polar angles ($w$) are investigated by comparing the particle size descriptors (including volume, surface area and principal dimensions) and the particle shape descriptors (including aspect ratios, sphericity, convexity and angularity index) calculated from the surfaces reconstructed using different $N$ and $w$ values. Correlations between different shape descriptors of the studied sands are then examined. Finally, a numerical algorithm utilizing the concept of principal component analysis (PCA) [28] and empirical cumulative distribution functions (ECDF) is proposed. Taking into account the intrinsic relationships among the SH coefficients at the first degree and the correlation between each evaluated SH coefficient, the proposed algorithm aims to regenerate realistic numerical particles based on the images obtained from 3D μXCT. Examined by comparing quantitatively the morphological features of the generated particles to those of the scanned ones, it is concluded that the proposed algorithm can successfully generate numerical particles which highly resemble the morphological features of the target sands.

## 2. Material tested, μXCT image acquisition and processing

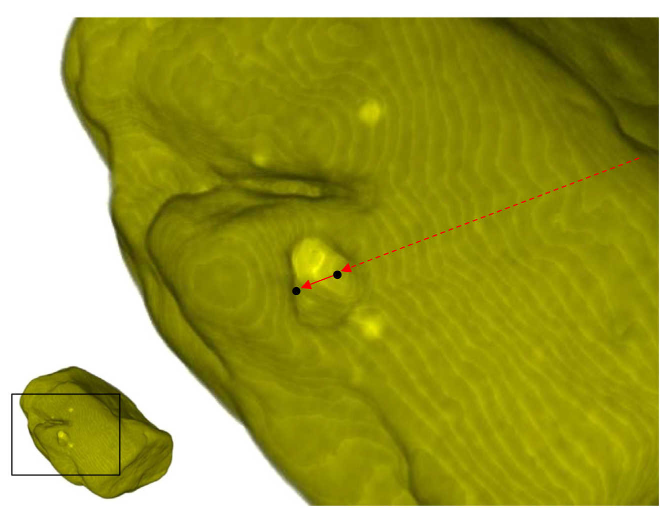
μXCT is a robust tool to study nondestructively the morphology and internal structure of materials [16,29–33]. The X-ray source of the device produces a polychromatic beam of X-ray photons passing through the scanned materials. Owing to the fact that different materials exhibit various amount of absorption, the attenuated X-ray, which is recorded using a detection device, reveals both the morphology and internal structure of the particles. By placing the studied materials onto a rotary table subject to X-ray, cross-sectional images (or slices) of the materials can be obtained which can be assembled into 3D images.

In this study, sand particles were scanned using the μXCT facility (XRadia Micro XCT-400) at the Shenzhen University, China. The studied sand is called the Pingtan Sand (PTS), which is a standard testing sand commonly used in China. Pingtan Sand is a natural, siliceous sand consisting of rounded to subrounded grains with a silica content of over 96%. A total of 104 PTS particles with sizes ranging from 1 to 2.8 mm were scanned in two separate batches. The sand particles were first placed in a plastic tube with inner diameter and height both equal to 10 mm. Each particle was intentionally separated by transparent plastic sheets, which exhibit a much lower X-ray absorption rate than the sand particles, to avoid the needs of potential problematic particle segmentation during data processing [34]. A 1024 × 1024 pixel X-ray camera was used and the X-ray source was excited with a voltage of 139 keV and a current of 62 μA. The parameter settings were based on the sample geometry and the material composition [35] which aimed to achieve a resolution of 10 μm/voxel. Fig. 1(a) presents a 3D rendered view of a typical layer of sand particles, while Fig. 1(b) shows a local view of a PTS particle that owns a concave void on the surface. The void makes that some piece of the particle's surface cannot be described by a star-shaped particle due to the reentrance problem.

As shown in Fig. 2, the images obtained from μXCT scanning were further partitioned such that each stack of the partitioned images only recorded one single particle. Each image file in the stack was then processed by a 3D 2 × 2 × 2 median filter to reduce the noise level of the raw images [17,36]. As the absorption rate of the plastic sheet is distinctively lower than that of the sand particle, the plastic sheet can be easily removed from the sand particle by traditional image binarization. In this




(a) a layer of sand particles



(b) reentrance problem associated with a concave void

**Fig. 1.** 3D visualization of typical sand particles.