Micromorphology characterization and reconstruction of sand particles using micro X-ray tomography and spherical harmonics

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Abstract

The particle micromorphology created by geological processes is an essential characteristic in determining the mechanical properties of natural sands. Based on micro X-ray computed tomography (\(\mu\)CT) data, we introduce a mathematical procedure using spherical harmonics to characterize and reconstruct the particle micromorphology in three dimensions. The basic geometric properties of natural sand particles, volume and surface area, and two empirical engineering indices, sphericity and angularity, are the main focus of the investigation using spherical harmonic analysis. By validating the spherical harmonic analysis against the tomography data, it is shown to be a robust technique for reproducing particle micromorphology in terms of the shape irregularity and surface texture. The precision of the method depends on the resolution of the \(\mu\)CT and the maximum harmonic degree used. Finally, by using principal component analysis for spherical harmonic descriptors of the scanned particles, two different kinds of sand assemblies consisting of statistically reconstructed particles with random shapes but major morphological features are successfully generated. This approach will be useful for the efficient discrete element modeling of real sands in the future.

1. Introduction

Particle micromorphology, such as the shape irregularity and surface texture, is important in understanding the geological origin and geomechanics of natural rock and sand, and as such has been of interest to both geological and geotechnical engineers for many decades. Specifically, surface textures observed by scanning electron microscopy clearly reveal the geological setting and weathering processes of the particle (Sharp and Gomez, 1986; Krinsley and Marshall, 1987). A great deal of experimental study has shown that the macroscopic mechanical properties of sands, such as the shear strength, dilatancy, crushability, and shear-induced localization, are highly influenced by the inherent fabric and shape of the particle (Coop et al., 2004; Guo and Su, 2007; Tsomokos and Georgiannou, 2010; Fityus et al., 2013).

As an alternative to investigating fundamental soil behavior, the discrete element method (DEM), first proposed by Cundall and Strack (1979), has made significant contributions towards unraveling the micromechanical mechanisms of particle micromorphology that affect the mechanical properties of sands. Two major developments in this line of research should be highlighted: DEM-based clump logic to model shape irregularities (Matuttis et al., 2000; Mahmood and Iwashita, 2011) and the rolling resistance contact model to represent surface textures (Iwashita and Oda, 2000; Jiang et al., 2005). From a microscopic point of view, shape irregularity and surface texture are thought of as the physical sources of the interlocking force and frictional roughness related to particle-scale kinematics during the quasi-static shearing of sands. The micromechanics of the anti-rotation effects induced by irregular shape and surface texture have previously been investigated by the authors (Zhou et al., 2013).

In this context, the quantitative characterization and reconstruction of particle micromorphology hold the key to further studies in both geological and geomechanical research. Traditionally, it has been convenient for engineers to measure some of the morphological parameters of particles (e.g., sphericity and roundness) by comparing the microscopic view with the standard chart provided by Krumbein and Sloss (1963). Other morphological parameters, such as size, aspect ratio, and convexity, and their statistical distributions can be automatically analyzed using the QICPIC laser scanner (Sympatec, 2008). Due to the multiscale nature of particle morphology, a fractal dimension has been used to depict the self-similar characteristics of surface texture and roughness details at different length scales (Vallejo, 1995; Hyslip and Vallejo, 1997; Kolay and Kayabali, 2006). Each of these parameters may provide information about certain aspects of particle morphology, but they have significant degrees of inaccuracy and variance due to the two-dimensional (2-D) representation of particle morphology by the microscope. The development of X-ray micro-computed tomography (\(\mu\)CT) technology provides a powerful tool for the quantification and reconstruction of the three-dimensional (3-D) characteristics of natural sands. Early use of the CT technique on granular soils focused mainly on
the characterization of the particle kinematics and deformation localization during the shearing process (Hall et al., 2010; Hansan and Alshibli, 2010). Recently, enhancements to μCT resolution have allowed the detection and identification of the internal microstructures (e.g., joints and fissures) and minerals of the rock mass (Yun et al., 2013), and individual particle micromorphology and the interparticle contact geometries of sands (Fonseca et al., 2012, 2013; Uday et al., 2013). Using a variety of image processing techniques, the previously mentioned morphological parameters can also be obtained, becoming more meaningful and precise within the 3-D scenario.

As a single descriptor gives only limited information about the morphological features of a particle, a large set of descriptor indices are always needed to plot a relatively comprehensive figure of particle micromorphology. For example, using QICPIC analysis, a long list of indices representing different particle properties can be evaluated. Even so, it is still difficult to reconstruct a realistic particle micromorphology, no matter how many descriptors are used as the input. In addition, two major disadvantages commonly exist in the application of traditional characteristic descriptors. The definitions are artificial and hard to unify for different research settings (Fonseca et al., 2012) and the computing and storage resources required for the used image dataset are extremely large, especially for enhanced μCT. To overcome these limitations, it is important and necessary to put forward a uniform descriptor that is able to reconstruct particle micromorphology in 3-D space. Bowman et al. (2001) first introduced the mathematical Fourier descriptors to characterize and reconstruct particle micromorphology in 2-D space. This method was then extended to 3-D space by Mollon and Zhao (2013) to reconstruct a sand particle through three orthogonal cross-sections of the original surface profile. However, the intrinsic drawback of this method is that some local information about the surface morphology will be lost by the artificial choice of these cross-sections, especially for highly irregular particles.

As an alternative mathematical approach, spherical harmonic (SH) series, the 3-D extension of the Fourier series, is introduced in this study to develop the characterization and reconstruction of particle micromorphology. This method has recently received a lot of attention, and has been widely applied to many fields, for example, in the investigation of organ pathology using biomedical image analysis (Gerig et al., 2001; Chung et al., 2008), the identification and reconstruction of morphological structure in bioinformatics (Shen and Makedon, 2006; Shen et al., 2009a), and topography surveying in geophysics and astronomy (Zuber et al., 2000; Bucha and Janák, 2013). The earlier application of SH analysis in geological and geotechnical engineering was only capable of reconstructing star-shaped (i.e., convex) objects. For example, by expanding the polar radius from a standard sphere, Garboczi and his co-workers (Garboczi, 2002; Taylor et al., 2006) successfully developed the use of SH analysis for convex concrete aggregates. However, surface non-convexity induced by weathering and erosion is a basic feature of natural sand (Krinsley and Marshall, 1987), and should be considered in the characterization and reconstruction of particle micromorphology. A similar difficulty was also faced by biomedical scientists reconstructing brain structures using the traditional SH expansion (Shen et al., 2009b). Therefore, Brechbühler et al. (1995) proposed that the surface profile of a non-convex object could be represented by three simultaneous Cartesian coordinate functions expanded by SH series, which is highly applicable for natural sand particles.

In this study, we firstly introduced the basic framework of the μCT image processing and the SH analysis for the characterization and reconstruction of the particle micromorphology of natural sand. The SH-based functions were then used to calculate the basic particle properties (i.e., volume and surface area) and to validate the applicability and accuracy of this mathematical approach. Finally, based on the principal component analysis (PCA) of the obtained SH descriptors, two types of random-shaped particle assemblies, including...
2. Methodology

2.1. Image processing of the μCT data

Leighton Buzzard sand (LBS) and highly decomposed granite (HDG), were reconstructed and the statistical features of their particle micromorphology were investigated.

LBS has been widely used in research as a standard quartz sand for many years. It is quarried locally around the town of Leighton Buzzard in southeast England from the lower Greensand sequence, which was deposited in shallow sea and estuarine environments. Its particles are rounded and smooth as can be seen in the microscope view of Fig. 1(a), and this may result from geological transportation processes. The mineralogy is predominantly quartz with some feldspar (Sharp and Gomez, 1986). HDG, commonly found in Hong Kong, is mainly derived from weathering and erosion of granitic rock outcrops. The particle micromorphology of HDG is always characterized by angularity, roughness, and non-convexity, as shown in Fig. 1(d). Eight LBS particles and four HDG particles were randomly picked from the screening packing, with the particle size from 1.18 mm to 2.36 mm. These selected particles were fixed in a microtube with silicon oil and then scanned by a Phoenix nanome|x using a resolution of 10 μm at the Advanced Engineering Material Facility (AEMF) of the Hong Kong University of Science and Technology. A 3-D gray matrix was obtained after the X-ray scanning to provide a full picture of the particle, including the internal microstructures and surface micromorphology. In this study, the main objective of processing the original scanning data was to capture information of the shape irregularity and surface texture of the sand particles.

Data preparation for the SH analysis included three major stages of image processing. First, the images were segmented and partitioned into regions of individual particles and silicon oil. By setting an appropriate value as the intensity threshold of the attenuation associated with each voxel, the segmentation was used to label each voxel as either silicon oil or solid particle. Second, the intrinsic function bwperim in MATLAB (Mathworks, 2010) was used to identify the boundary voxels of each individual particle. Within each tomography of the particle, a given non-zero voxel connecting with at least one zero voxel was detected as a part of the boundary. Considering the complex morphology of HDG particles, the face plus edge adjacent algorithm was used to determine the connectivity between the non-zero and zero voxels. Subsequently, one set of boundary voxels of an individual particle was obtained and allocated to an independent binary image. Based on the resolution of the μCT and a given reference coordinate, the spatial map of the surface micromorphology was then established in the Cartesian space in terms of a set of vertices and faces, as visualized in Fig. 1(b) and (e). Meanwhile, all the 3-D images of the scanned particles were summarized in Fig. 2. It is distinct that HDG particles appear much more irregular and rough than LBS particles.

Finally, the most important step, spherical topology fixing, was conducted based on the morphological map of each particle. Shen and Makedon (2006) emphasized that the necessary condition for SH analysis was topological invariance and not continuous convexity. Geometrically, this means that the object topology can be transformed into a standard sphere by a series of continuous deformations (e.g., scaling and warping). In accordance with this approach, the boundary noise of the particle morphology map, including internal holes, non-connective edges, and vertices, needs to be detected and removed. Fig. 1(c) and (f) shows the results of selected LBS and HDG particles after topological repair. It is clear that the topological fixing of HDG01 displays a much more distinct effect than that of LBS01. This is due to a large number of fragments attached with weak clay minerals by weathering to the HDG particle surface.

2.2. Spherical harmonic analysis

After the image processing of the μCT data, a set of surface vertices with Cartesian coordinates, \( V(x, y, z) \), of a given particle was obtained. To obey the principle of simultaneous control of area and length distortion (Shen and Makedon, 2006), spherical parameterization was performed to create a bijective mapping from the surface profile to a unit sphere. As a result, a set of surface points \( V \) was obtained, associated with the corresponding spherical coordinates.
Taking the parameterized surface points $V(\theta, \phi)$ as the input on the left-hand side of Eq. (2), this equation can be extended to a matrix form,

$$
\begin{pmatrix}
\begin{bmatrix} y_1^n & y_2^n & \ldots & y_{n+1}^n \end{bmatrix} - y_0^n \end{pmatrix} = \begin{pmatrix} T_x & T_y & T_z \end{pmatrix}, \quad \text{(6)}
$$

where $Z = \begin{pmatrix} y_1^n & y_2^n & \ldots & y_{n+1}^n \end{pmatrix}$ is reshaped from a triangle matrix to a row vector, in which $\theta$ and $\phi$ are the $i$th pair of the spherical coordinates of the particle surface points $V(\theta, \phi)$. Correspondingly, the matrix form of $c_i^n$ was also reshaped to $c = \begin{pmatrix} c_1^2 & \ldots & c_{n+1}^2 \end{pmatrix}$ in a similar way but transposed to a column vector.

For one set of $c_i^n$, a total of $(n+1)^2$ unknown coefficients need to be determined by $i$ linear equations in Eq. (6). There will be solutions if $i$ is equal to or bigger than $(n+1)^2$. Generally, the number of parameterized surface points $i$ is large enough to meet the precision requirement for most scientific problems. Meanwhile, $n_{\text{max}} = 12$ is enough for most engineering applications (Garboczi, 2002).

Adopting matrix right division to perform the standard least squares estimation using Eq. (7), it is easy to solve these linear equations and determine all of the coefficients of $c_i^n$.

$$
c = Z \big/ V \quad \text{(7)}
$$

Now, $c_i^n$ can be used as the characteristic descriptor for the reconstruction of the particle micromorphology based on Eq. (2).

2.3. Evaluation of particle properties using spherical harmonic functions

Using the surface coordinate functions $V(\theta, \phi)$ obtained previously, it is desirable to calculate the basic characteristics of the sand particles, such as surface area and volume. For both convex and non-convex particles, it is possible to divide the object space into a mass of infinitesimal hexahedral elements. The position vector of any surface element from the particle center $\vec{r}(\theta, \phi)$ is expressed as

$$
\vec{r}(\theta, \phi) = V(\theta, \phi) - V_0 \big/ V, \quad \text{(8)}
$$

where $V_0 = (x_0, y_0, z_0)^T$ is the particle center given by the zero degree expansion of Eq. (2) (i.e., $n = 0$).

Randomly take one hexahedral element for analysis, as illustrated in Fig. 3. Along the polar direction of $\vec{r}(\theta, \phi)$, the position vector of the element can be expressed as $\alpha \vec{r}(\theta, \phi)$, in which $0 \leq \alpha \leq 1$ is an interpolated coefficient representing the spatial location of the element within the particle. After determining $\vec{r}(\theta, \phi)$, the edge vectors of the hexahedral element can then be easily obtained, as illustrated in Fig. 3. Note that the directions of these edge vectors apply to both convex and non-convex features, which will be encountered in the evaluation of sand particle characteristics. According to the geometrical definition of the mixed product of these edge vectors, the volume of the hexahedral element can be expressed as

$$
dV = \left( \frac{\partial r_x}{\partial \theta} \times \frac{\partial r_y}{\partial \phi} \right) \cdot d\alpha \vec{r} \big/ r. \quad \text{(9)}
$$

Integrating Eq. (9) yields

$$
V = \int_0^1 \int_0^{\pi} \int_0^{\pi} \left( \frac{\partial r_x}{\partial \theta} \times \frac{\partial r_y}{\partial \phi} \right) d\alpha d\theta d\phi \cdot d\alpha \vec{r}. \quad \text{(10)}
$$
The validation of the SH analysis was made by comparing the mathematical predictions with the theoretical or image-based results of one standard cubic and two sand particles, LBS02 and HDGO2, selected from the particle assembly. For each particle, the coefficients $c^n_m$, called the SH descriptors, were obtained from the SH expansion discussed previously. This set of $c^n_m$ was then used for the validation in two steps: 1) reconstructing and visualizing the particle micromorphology; and 2) computing the particle geometric

Furthermore, using the above results of particle volume and surface area, the previously mentioned sphericity index ($SI$) can be calculated as:

$$SI = \frac{\sqrt{36nV^2}}{S}.$$  \hfill (16)

Another important engineering parameter, the average angularity index ($AI$), can also be conveniently evaluated using Eq. (17), although it is difficult to evaluate this parameter based on the image results.

$$AI = \frac{s^2}{2n^2} \sum_{\theta=0}^{\pi} \sum_{\phi=0}^{\pi} |r_P - r_{EE}|.$$  \hfill (17)

where $s$ is the detecting step, set to 0.01 $\pi$ in this study, $r_P$ is the polar radius with the spherical coordinate $(\theta, \phi)$, and $r_{EE}$ is the polar radius of the equivalent ellipsoid with the spherical coordinate $(\theta, \phi)$. The equivalent ellipsoid can be easily obtained by the first degree expansion of the SH series. Note that Eq. (17) is a 3-D extension of the 2-D definition of the particle angularity index in ASTM D5821 (2006).

These two engineering parameters are commonly used to evaluate the morphological features of sand particles. However, while $SI$ is linked more to the shape irregularity, $AI$ is linked more to the surface texture.

### 3. Results and discussions

#### 3.1. Validation of spherical harmonic analysis

The validation of the SH analysis was made by comparing the mathematical predictions with the theoretical or image-based results of one standard cubic and two sand particles, LBS02 and HDGO2, selected from the particle assembly. For each particle, the coefficients $c^n_m$, called the SH descriptors, were obtained from the SH expansion discussed previously. This set of $c^n_m$ was then used for the validation in two steps: 1) reconstructing and visualizing the particle micromorphology; and 2) computing the particle geometric

<table>
<thead>
<tr>
<th>Image view</th>
<th>$n = 1$</th>
<th>$n = 5$</th>
<th>$n = 10$</th>
<th>$n = 20$</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a)</td>
<td>(b)</td>
<td>(c)</td>
<td>(d)</td>
<td>(e)</td>
</tr>
</tbody>
</table>

Fig. 4. SH reconstructions of particle micromorphology with different SH degrees $n$: (a) image view, (b) at $n = 1$, (c) at $n = 5$, (d) at $n = 10$, and (e) at $n = 20$. 

of 20, in the current study, was generally found to be sufficient for the morphological reconstruction of major features of shape irregularity and surface texture, even for the highly irregular HDG particles.

Based on Eqs. (12) and (15), the volume and the surface area of these three particles as a function of the SH degree \( n \) were examined in detail, as shown in Fig. 5. It was found that the particle volume (Figure 5a) converged rapidly to a stable value that matched the image processing result after \( n > 10 \), but an apparent under-prediction with a roughly 11% difference from the image-measured value was found for particle HDG02. The image-measured and SH-predicted results with a fixed \( n \) of 10 of all the scanned particles are summarized in Table 1. It was seen that the difference in volume from the image-measured value was less than 1.2% for all LBS and HDG particles, while the difference (under prediction) in surface area from the image-measured value ranged between 10% and 30% for all HDG particles, although it also remained under 1.2% for all LBS particles.

The above difference in surface area between the image-measured and SH-predicted values is mainly attributed to the high surface roughness of HDG particles, which affects little the particle volume but significantly the particle surface area. The SH analysis, essentially being a curve-fitting method, produces a mathematically continuous surface profile which allows an excellent estimate of a 3-D property like volume but less accurate estimate of a 2-D property like surface area with the same SH degree \( n \) used. Theoretically, however, it is possible to achieve a better agreement with the image-measured value by employing a higher SH degree. In fact, the trend of the surface area curve of HDG02 in Fig. 5b does not seem to converge and still slowly approaches the image-measured value at \( n = 20 \). However, it is undesirable to make such a refined SH analysis for most geological and geomechanical problems for two reasons: 1) the high degree analysis is very computationally expensive and unaffordable for large-scale problems involving a huge number of soil particles; and 2) the image-measured value may itself contain some errors due to the adjacent algorithm used to identify the boundary voxels of the particle image. Regarding the second reason, the source of the error is caused by possible different treatments of voxel connectivity e.g., face or edge adjacency, in the boundary detection process, and indeed it is impossible to know the “true” surface area just based on the tomography images with a limited resolution. Such a problem was also reported by Fonseca et al. (2012), who found that the image-measured surface area of a standard microsphere had a 30% over-prediction than its theoretical value.

Fig. 6 shows the correlation between the sphericity index SI and the angularity index AI of all the particles evaluated using Eqs. (16) and (17). It is clear that a negative linear correlation, as shown in Eq. (18), exists between SI and AI for all the sand particles, although the HDG data exhibit more scatter than LBS data due to again the higher levels of shape irregularity and surface roughness of HDG particles.

\[
AI = -0.714SI + 0.774 \tag{18}
\]

The LBS particles have generally higher SI but lower AI values than HDG particles, as expected. Meanwhile, it is interesting to note that

<table>
<thead>
<tr>
<th>Particle no.</th>
<th>Volume</th>
<th>Image process</th>
<th>Spherical harmonic</th>
<th>Difference (%)</th>
<th>Surface area</th>
<th>Image process</th>
<th>Spherical harmonic</th>
<th>Difference (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>LBS01</td>
<td>2.817</td>
<td>2.851</td>
<td>1.136</td>
<td>10.21</td>
<td>10.33</td>
<td>1.1253</td>
<td></td>
<td></td>
</tr>
<tr>
<td>LBS02</td>
<td>3.219</td>
<td>3.236</td>
<td>0.522</td>
<td>11.86</td>
<td>11.78</td>
<td>0.8233</td>
<td></td>
<td></td>
</tr>
<tr>
<td>LBS03</td>
<td>2.429</td>
<td>2.453</td>
<td>0.988</td>
<td>10.01</td>
<td>9.902</td>
<td>0.1256</td>
<td></td>
<td></td>
</tr>
<tr>
<td>LBS04</td>
<td>1.918</td>
<td>1.940</td>
<td>1.126</td>
<td>9.094</td>
<td>9.075</td>
<td>0.2067</td>
<td></td>
<td></td>
</tr>
<tr>
<td>LBS05</td>
<td>2.173</td>
<td>2.178</td>
<td>0.021</td>
<td>9.733</td>
<td>9.792</td>
<td>0.6093</td>
<td></td>
<td></td>
</tr>
<tr>
<td>LBS06</td>
<td>1.895</td>
<td>1.917</td>
<td>1.150</td>
<td>8.589</td>
<td>8.579</td>
<td>0.1153</td>
<td></td>
<td></td>
</tr>
<tr>
<td>LBS07</td>
<td>2.380</td>
<td>2.398</td>
<td>0.757</td>
<td>9.726</td>
<td>9.676</td>
<td>0.5151</td>
<td></td>
<td></td>
</tr>
<tr>
<td>LBS08</td>
<td>2.084</td>
<td>2.102</td>
<td>0.869</td>
<td>8.491</td>
<td>8.480</td>
<td>0.1319</td>
<td></td>
<td></td>
</tr>
<tr>
<td>HDG01</td>
<td>11.31</td>
<td>11.30</td>
<td>-0.008</td>
<td>43.86</td>
<td>31.39</td>
<td>-28.43</td>
<td></td>
<td></td>
</tr>
<tr>
<td>HDG02</td>
<td>3.065</td>
<td>3.051</td>
<td>0.084</td>
<td>13.78</td>
<td>12.31</td>
<td>-10.67</td>
<td></td>
<td></td>
</tr>
<tr>
<td>HDG03</td>
<td>5.463</td>
<td>5.486</td>
<td>0.604</td>
<td>21.67</td>
<td>17.19</td>
<td>-20.67</td>
<td></td>
<td></td>
</tr>
<tr>
<td>HDG04</td>
<td>6.380</td>
<td>6.371</td>
<td>0.368</td>
<td>24.40</td>
<td>21.12</td>
<td>-13.44</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Fig. 5. Particle volume and surface area of the normal cube LBS02 and HDG02 as a function of the SH degree \( n \), (a) volume and (b) surface area.
the standard sphere and the ellipsoid deviate significantly from the correlation line but the standard cube fits the line very well. This indicates that these two indices are well correlated for irregular non-sphere-like particles and not for idealized sphere-like particles.

3.2. Understanding the spherical harmonic descriptor

The standard cube in Fig. 4 is used in this section to illustrate the morphological features depicted by the SH descriptors. According to Eq. (2), it is easy to understand that the SH reconstruction of particle micromorphology is a cumulative process with the increase of the SH degree \( n \). Therefore, one can decompose the summing form of Eq. (2) into a series of independent frequency components, as expressed in Eq. (19):

\[
v_n(\theta, \varphi) = \sum_{m=-n}^{n} c_n^m Y_n^m(\theta, \varphi), \quad (n = 1, 2, \ldots, n_{\text{max}}).
\]

Note that \( v_n(\theta, \varphi) \) is a single point representing the particle center coordinate, which was excluded here to translate the particle center to the origin of the global coordinate system. The influence of different frequency components can be expressed by their amplitudes \( l_n \) of the corresponding SH coefficients as follows,

\[
l_x^n = \sqrt{\sum_{m=-n}^{n} |c_n^m|^2} ; \quad l_y^n = \sqrt{\sum_{m=-n}^{n} |c_n^m|^2} ; \quad l_z^n = \sqrt{\sum_{m=-n}^{n} |c_n^m|^2}.
\]

where \( l_x^n, l_y^n \) and \( l_z^n \) are the three orthogonal amplitude components of the \( n \)-degree frequency term, respectively, and \(|c_n^m|\), \(|c_n^m|\) and \(|c_n^m|\) are the three orthogonal norms of the SH descriptor of the \( n \)-degree frequency, respectively.

Fig. 7 shows the variations of three amplitude components as a function of the frequency degree \( n \) for the standard cube. It clearly shows that each amplitude component attenuates rapidly with the increase of degree \( n \), and become negligible after \( n \) exceeds 10. Fig. 8 shows the contour maps of the three Cartesian coordinate components of \( v_n(\theta, \varphi) \) (i.e., \( x_n(\theta, \varphi), y_n(\theta, \varphi) \) and \( z_n(\theta, \varphi) \)) at four selected ordinate spaces. It is seen that for \( n = 1 \) in Fig. 8a, the contour shapes are simplex and fluctuate in a large scale bar, representing the 2-D projection of the first degree ellipsoid shown in Fig. 4b. For \( n = 3 \) in Fig. 8b, features of alternating sub-peaks and sub-valleys depicting the prevailing convexities and non-convexities of the surface texture at a smaller length scale are observed. The general shape of the particle is captured by accumulating the first three degrees of SH descriptors. With an increase of \( n \) from 5 to 10 (Figure 8c and d), the contour

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**Fig. 6.** Correlation between the sphericity and angularity of the scanned LBS, HDG, and idealized particles.

**Fig. 7.** Frequency amplitude magnitudes as a function of the degree \( n \) for the three coordinate components.
maps exhibit increasingly complex patterns, with more frequent fluctuations in decreasing amplitudes. It seems that the surface texture of the particle morphology is almost formed from \( n = 5 \) to \( 10 \), with yet more roughness details at further smaller length scales to be included at larger \( n \) degrees. Based on the above results, we can divide the SH expansion series roughly into three stages fulfilling different functions, as shown in Fig. 7: 1) \( n = 1 \)–3 for the formation of the shape irregularity; 2) \( n = 3 \)–8 for the formation of the surface texture and 3) \( n \geq 9 \) for the formation of minor roughness details.

3.3. Statistical reconstruction of sand particle micromorphology

As mentioned before, an important advantage of the SH descriptor is its ability to reconstruct particle micromorphology, which will be of interest to many geological and geotechnical researchers. The reconstruction of realistic sand particles is the first step in advanced DEM simulations for the investigation of the effects of particle morphology on the micro- and macro-mechanical behaviors of sand (Ferellec and McDowell, 2010). However, the finite number of scanned particles cannot provide the full information required for such a one-to-one mapping in DEM simulations, which practically is also highly difficult and unnecessary. As an alternative, the statistical reconstruction of a sand assembly using SH descriptors obtained from a limited number of scanned particles is a novel and powerful approach to this goal. This is achieved through applying the principal component analysis (PCA) (Jolliffe, 2005) to the SH descriptors to derive the principal statistical variables for the morphology reconstruction.

It is evident from the SH analysis that a total number of \( 3(n + 1)^2 \) variables of a complete matrix of SH descriptor \( c^n \) is needed to reconstruct a particle. However, it is a difficult task to establish the

![Fig. 8. Fluctuation contour of the three coordinate components with different frequency degrees \( n \). (a) \( n = 1 \), (b) \( n = 3 \), (c) \( n = 5 \), and (d) \( n = 10 \).](image-url)
relationship between each variable of the descriptor matrix and the reconstructed particle morphology. The PCA is now made to reduce the dimensionality (i.e., number of variables) and yield the principal component variables of the descriptor matrix $c^m_n$. The PCA involves two major transformations for each particle: 1) the particle center must be translated to the origin of the global coordinate system and the original surface vertices must be rotated until the principal directions of its first degree ellipsoid are parallel to the global coordinate axes, as shown in Fig. 9; and 2) the particle volume must be scaled to the unit sphere. The updated SH descriptor $c^m_n$ of the transformed and normalized particle can then be obtained by Eqs. (6) and (7).

In this study, $c^m_n$ of all eight LBS particles and four HDG particles was obtained and used as the input of PCA. The major calculation can be readily completed by invoking the intrinsic built-in function `princomp` of MATLAB, yielding two important outputs, the principal component direction vectors $p$ and the corresponding variance coefficients $c_v$. Considering the major influence of the first three terms on the variance coefficients, the first three principal components were selected for particle morphology reconstruction in the current study. As such, the SH descriptor $\hat{c}$ of a reconstructed random-shaped particle can be expressed as:

$$\hat{c} = \bar{c} + p(x_1) \cdot c_v(x_1) \cdot x_2,$$

where $\bar{c}$ is the mean vector of previously obtained $c^m_n$ of all input particles, $x_1 \in \{1, 2, 3\}$ is the random number determining a random principal component $p(x_1)$ and the corresponding variance coefficient $c_v(x_1)$, and $x_2 \in [-3.0, 3.0]$ is a random real number which satisfies the Gaussian distribution and determines the variance intensity of the current principal component. Note that a larger range of $x_2$ will result in a greater degree of variance in the particle morphology reconstruction.

Fig. 10 shows two assemblies of statistically reconstructed sand particles containing 50 LBS and 50 HDG particles, respectively. As compared to the CT images of 12 original sand particles shown in Fig. 2, it can be observed that all the reconstructed particles resemble the mother particles in a way that they retain the major morphological features of the mother particles although each particle has a completely random shape. The assembly of LBS can be easily distinguished from that of HDG in that the latter appears much more irregular in terms of overall shape, surface texture and non-convex features. Due to the unavailability of more CT data of HDG particles at present, a lower degree of variance of the morphologies of reconstructed HDG particles than that of reconstructed LBS particles is observed. An improvement on this limitation can be made in the future when more CT data of HDG particles are available.

Fig. 11 shows the correlation between $SI$ and $AI$ for all the reconstructed LBS and HDG particles. The average values of $SI$ and $AI$ for the mother LBS and HDG particles, together with their range of variation are also plotted in Fig. 11 for comparison. Again, all the data were found to be nicely fit by a negatively sloped line, with reconstructed HDG data showing a larger amount of scatter than LBS data. These features are consistent with those observed for real sand particles previously. These results have demonstrated the effectiveness of PCA in the statistical reconstruction of irregular sand particles that contain the essential
morphological features of target sand particles. This approach will be a promising tool for advanced DEM simulations of real sands in the future.

4. Conclusion

The main point of this study was to introduce the use of SH analysis to characterize and reconstruct sand particle micromorphology in 3-D space. Based on μCT data from a series of image processing techniques, a set of coefficients called the SH descriptors can be obtained after surface parameterization and expansion. These SH descriptors could be used in a number of engineering applications. The main conclusions are summarized as follows.

SH expansion is a cumulative process used to ascertain the particle micromorphology, with three stages used to achieve representations of the shape irregularity, surface texture and roughness detail. The precision of the SH reconstruction relies strongly on the μCT resolution and the maximum SH degree used. For natural sand particles such as LBS and HDG, basic characteristics such as volume and surface area can be determined when the maximum SH degree is set near to 10. It is important to emphasize that surface area calculation by SH analysis can be thought of as the calibration of the image-measured result, especially for HDG particles, which have rich attachments and roughness details. Two advanced engineering parameters for the particle morphology (i.e., sphericity and angularity in 3-D) were conveniently evaluated by the SH analysis, and a strong linear relationship was found between them.

Statistically, by using PCA for the normalized SH descriptors of all scanned particles, different kinds of sand assembly with random-shaped particles can be reconstructed. This approach successfully shows the difference in the micromorphological characteristics of particles in terms of sphericity and angularity. The results presented in this paper demonstrate adequately the higher levels of theoretical rigor, completeness and modeling precision of the current approach over other traditional methods, such as QICPIC and fractal analyses, in the characterization and reconstruction of particle morphologies of granular materials. The further development of the current study will focus on the DEM sample reconstruction with realistic sand particles, which will reveal the interparticle micromechanics during quasi-static shearing. In addition, SH analysis based on an in situ process.
single particle crushing test accompanied by μCT scanning will greatly contribute to the understanding of the micromorphological evolution of natural sand particles induced by external loads and geological weathering.

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Appendix 1. Derivations of the spherical harmonic functions

Using $x_0$ and $x_\phi$ for the purpose of demonstration and substituting Eq. (3) into Eq. (2), the SH expansion for the $x$ component can be expressed as:

$$x(\theta, \phi) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} c_{nm} \sin^n \theta \cos^m \theta e^{im\phi}. \tag{22}$$

Differentiating both sides of Eq. (22) with respect to $\theta$, we have,

$$\frac{\partial x(\theta, \phi)}{\partial \theta} = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \frac{n}{\sin \theta} c_{nm} \sin^{n-1} \theta \cos^n \theta \cos^m \theta e^{im\phi}, \tag{23}$$

where, according to the recurrence relation of associated Legendre functions expressed in Eqs. (4) and (5), we have,

$$\frac{\partial P_n^m (\cos \theta)}{\partial \theta} = -\frac{1}{\sin \theta} \left[ (n+1) \cos^m \theta P_n^{m-1} (\cos \theta) - (n-m+1) P_n^{m+1} (\cos \theta) \right]. \tag{24}$$

Therefore, $x_\theta$ can be rewritten as,

$$x_\theta = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \frac{n}{\sin \theta} c_{nm} \sin^{n-1} \theta \cos^n \theta \cos^m \theta e^{im\phi}. \tag{25}$$

Differentiating both sides of Eq. (22) with respect to $\phi$, we obtain

$$x_\phi = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} (im)e^{im\phi} \left[ \frac{2n+1}{4m(n+m)!} (n-m)(m+n+1)c_{nm} \cos^n \theta \sin^m \theta \right], \tag{26}$$

where $i$ is the imaginary unit.

All of the derivations in Eqs. (12) and (15) can be similarly obtained using the above formulations.

References


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