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A Simple Method for Particle Shape Generation with Spherical Harmonics

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1 **Abstract**

2 The increasing interest in particle shape influence on granular mechanics
3 necessitates a fast and robust particle shape generation method. We describe a new
4 approach based on rotation-invariant spherical harmonic (SH) analysis. The core of
5 this method is to construct morphology features at various length scales and
6 superimpose them together to form the overall morphology. This method uses four
7 rotation-invariant SH factors to construct SH coefficient matrices. We quantify
8 particle shape at form, roundness, and compactness to establish the linkage between
9 SH factors and traditional shape parameters. It is found that SH factors effectively
10 control particle features at different scales. This method has a great potential to
11 facilitate the research on granular mechanics considering particle shape effects.

12

13 **Keywords**

14 Compactness; form; particle morphology; particle generation; roundness; spherical
15 harmonics.

16 **1. Introduction**

17 Particle morphology influences both mechanical and flow behavior of granular
18 materials. For example, angular sands tend to have high shear strength (Cho et al.,
19 2006, Ashmawy et al., 2003), stress concentration at contacts (Zhao et al, 2015; Wang
20 and Coop, 2016), and resistance to flow and liquefaction (Cleary and Sawey, 2002,
21 Antony and Kuhn, 2004). Also, particle morphology influences particle interactions
22 with fluid and air, e.g., drag coefficient and mineral floatability (e.g., Haider and
23 Levenspiel, 1989; Xia, 2017). Therefore, particle shape is an important parameter to
24 predict and control the engineering properties of granular materials.

25 Recent years have witnessed a growing interest in representing particle shapes with
26 mathematical methods. Optical microscopy, laser beam systems, digital holography
27 and X-ray computed tomography have been used to obtain the morphology of
28 particles (e.g., Altuhafi et al., 2012; Wu et al., 2016; Zhao and Wang, 2016). Real
29 particle shapes can be effectively characterized and reconstructed at two-dimensional
30 (2D) with Fourier analysis (e.g., Bowman et al., 2001) and at three-dimensional (3D)
31 with spherical harmonic (SH) analysis (e.g., Garboczi, 2002; Zhou et al., 2015; Zhou
32 and Wang, 2016; Zhou et al., 2017; Garboczi and Bullard, 2017). Meanwhile,

1 mathematical methods have shown great potential for particle shape generation. For
2 example, Mollon and Zhao (2012) proposed an inverse operation to generate 2D
3 particle shapes with given Fourier descriptors. They later extended the method to the
4 3D case based on 2D contours (Mollon and Zhao, 2013) and discrete random field
5 (Mollon and Zhao, 2014). However, it remains a challenge to perform an inverse
6 operation using SH analysis, i.e., to construct SH coefficient matrices for a particle
7 with specified features.

8 In this study, we propose a simple method to generate 3D particle shapes with
9 prescribed shape features using SH analysis. There are five sections in the following
10 part of this paper. Section 2 briefly introduces the research background, including
11 particle shape quantification method (Zhao and Wang, 2016) and rotation-invariant
12 SH analysis (Zhao et al., 2017). Section 3 discusses the method to construct SH
13 matrices with given SH factors. Section 4 shows the examples of generated particles
14 and their shape quantification results. Section 5 discusses the advantage and
15 disadvantage of the current method and provides a summary of this study.

16

17 **2. Particle shape quantification and rotation-invariant SH analysis**

18 **2.1 Particle shape quantification**

19 Particle shape is complicated to quantify due to its multi-scale nature. This study
20 follows the particle shape quantification method proposed by Zhao and Wang (2016).
21 Six shape parameters are calculated to quantify form, roundness, and compactness, as
22 follows:

23 **Form (EI , FI , and AR)** As shown in Fig. 1(a), a 3D particle has three principal
24 dimensions, $p_1 \geq p_2 \geq p_3$, determined by the principal component analysis (PCA). For 3D
25 particles, particle form refers to two aspect ratios, namely elongation index ($EI = p_2/p_1$)
26 and flatness index ($FI = p_3/p_2$). Their mean value is referred to as the characteristic
27 aspect ratio (AR).

28 **Roundness (R_M)** Surface simplification is used to eliminate the influence of finer
29 shape features (e.g., roughness) on particle roundness index. Particle roundness is
30 quantified with the local curvature distribution at a particle surface with 1280
31 triangular elements. Zhao and Wang (2016) showed that surface roughness is
32 effectively removed and particle corners are well identified with this level of surface
33 simplification. Fig. 1(b) shows the distribution of mean curvature at particle corners.

1 Particle corners have larger curvature values than that of the particle's maximum
 2 inscribed sphere. Then, mean-curvature roundness index (R_M) is evaluated at the
 3 corners by the area-weighted average local mean curvature.

4 **Compactness (S and C_X)** Sphericity (S) describes how a particle is close to a
 5 sphere: $S = \frac{\sqrt[3]{36\pi V^2}}{SA}$, where V is particle volume, and SA is particle surface area. It

6 compares the surface area of a particle and its volume-equivalent sphere (Fig. 1c).
 7 Convexity reflects how closely a particle represents a convex hull. This parameter is

8 defined as $C_X = \frac{V}{V_{CH}}$, where V is particle volume and V_{CH} is the volume of its

9 convex hull. Fig. 1(d) illustrates convex hull in two-dimension.

10 **2.2 Rotation-invariant SH analysis**

11 Spherical harmonics are a complete set of orthogonal functions defined on the
 12 surface of a sphere. This method originally used a radial representation, which is
 13 restricted to star-shaped surfaces. Brechbühler et al. (1994) solved this limitation by
 14 introducing surface parameterization. Surface parameterization decomposes a 3D
 15 particle surface onto three orthogonal directions. It also enables establishing a linkage
 16 between SH coefficients and classical shape parameters (Zhao et al. 2017).

17 **2.2.1 Surface parameterization**

18 Surface parameterization creates a continuous and uniform mapping from particle
 19 surface to a unit sphere. Spherical parameterization results in a bijective mapping
 20 between each point on a surface and a pair of spherical coordinates:

$$21 \quad \mathbf{v}(\theta, \phi) = (x(\theta, \phi), y(\theta, \phi), z(\theta, \phi))^T, \quad (1)$$

22 where $(x(\theta, \phi), y(\theta, \phi), z(\theta, \phi))^T$ is the Cartesian coordinates of a vertex, while $\theta \in [0, \pi]$
 23 and $\phi \in [0, 2\pi]$ are the latitudinal and longitudinal coordinates, respectively.

24 **2.2.2 Spherical harmonic expansion**

25 The coordination of the vertices on a particle surface could be represented by
 26 spherical harmonic expansion as:

$$\begin{pmatrix} x(\theta, \phi) \\ y(\theta, \phi) \\ z(\theta, \phi) \end{pmatrix} = \begin{pmatrix} \sum_{l=0}^{l_{\max}} \sum_{m=-l}^l c_{x,l}^m Y_l^m(\theta, \phi) \\ \sum_{l=0}^{l_{\max}} \sum_{m=-l}^l c_{y,l}^m Y_l^m(\theta, \phi) \\ \sum_{l=0}^{l_{\max}} \sum_{m=-l}^l c_{z,l}^m Y_l^m(\theta, \phi) \end{pmatrix}, \quad (2)$$

where Y_l^m and $(c_{x,l}^m, c_{y,l}^m, c_{z,l}^m)$ are the spherical harmonic and coefficients of degree l and order m , respectively. The definition of Y_l^m follows Press et al. (1992). l_{\max} is the maximum SH degree used to reconstruct a particle surface.

SH analysis decomposes particle shape features into different SH degrees. For example, the shape features at an SH degree of l are characterized by:

$$\begin{pmatrix} x_l(\theta, \phi) \\ y_l(\theta, \phi) \\ z_l(\theta, \phi) \end{pmatrix} = \begin{pmatrix} c_{x,l}^{-l} & c_{x,l}^{-l+1} & \dots & c_{x,l}^l \\ c_{y,l}^{-l} & c_{y,l}^{-l+1} & \dots & c_{y,l}^l \\ c_{z,l}^{-l} & c_{z,l}^{-l+1} & \dots & c_{z,l}^l \end{pmatrix} \begin{pmatrix} Y_l^{-l}(\theta, \phi) \\ Y_l^{-l+1}(\theta, \phi) \\ \dots \\ Y_l^l(\theta, \phi) \end{pmatrix} = \mathbf{C}_l \mathbf{Y}_l(\theta, \phi), \quad (3)$$

where \mathbf{C}_l is a $3 \times (2l+1)$ -dimensional matrix including the SH coefficients of degree l . \mathbf{C}_0 only influences particle position, which is not considered in this study. For l greater than zero, \mathbf{C}_l contributes to finer shape features with increasing l . Specifically, \mathbf{C}_1 determines an ellipsoid, which is referred to as the first-degree ellipsoid (FDE).

2.2.3 Rotation-invariant SH analysis

Our previous study has defined two kinds of rotation-invariant factors from SH coefficients, i.e., spherical descriptors and their principal components (Zhao et al., 2017). These factors are only influenced by particle shape, not by particle position and rotation. Spherical descriptors are defined as:

$$d_l = \|\mathbf{C}_l\|_F = \sqrt{\sum_{i \in (x,y,z)} \sum_{m=-l}^l \|c_{i,l}^m\|^2} = \sqrt{\sum_{i \in (x,y,z)} \sum_{m=-l}^l c_{i,l}^m c_{i,l}^{m*}}, \quad (4)$$

where $\|\mathbf{g}\|_F$ is the Frobenius norm and $*$ denotes the conjugate transpose. Parseval's theorem indicates that spherical descriptors are correlated with the mean squared distance (MSD) from particle surface to the origin: $\sum_l d_l^2 = 4\pi \cdot \text{MSD}$.

Spherical descriptors tend to decrease linearly with increasing SH degree in a

1 log-log scale. Fig. 2(a) shows the results obtained from 80 Leighton Buzzard sand
 2 (LBS) particles (Zhao et al., 2017). The spherical descriptors are normalized by d_1 to
 3 eliminate the influence of particle size. The average values of spherical descriptors
 4 tend to follow power-law equations:

$$5 \quad \begin{cases} d_l = d_2 \cdot \left(\frac{2}{l}\right)^\alpha & \text{for } l \in [2, 8] \\ d_l = d_9 \cdot \left(\frac{9}{l}\right)^\beta & \text{for } l \in [9, 15] \end{cases} \quad (5)$$

6 The fitted values of α and β are 1.387 and 1.426, respectively. Zhao et al. (2017)
 7 showed that major shape features (e.g., form, roundness and compactness) are well
 8 characterized with SH degrees up to eight. Therefore, we define two sections in Eq. (5)
 9 to control different shape scales (i.e., roundness and roughness), although a single
 10 function could also fit well the descriptors. This correlation holds for any 40 randomly
 11 chosen particles with α and β in [1.320, 1.448] and [1.190, 1.672]. Zhao et al. (2017)
 12 show that similar correlations exist for LBS fragments that are more irregular than
 13 LBS particles. It is anticipated that these correlations also exist for other kinds of
 14 particles with different values of α and β . Then, the particles are aligned by rotating
 15 all the particles according to FDE, making p_1 , p_2 and p_3 corresponding to x -, y - and
 16 z -axes, respectively. Therefore, the spherical descriptors are decomposed as

17 $d_{i,l} = \sqrt{\sum_{m=-l}^l c_{i,l}^m c_{i,l}^{m*}}$ for i in (x, y, z) . Fig. 2(b) shows the mean values of $d_{i,l}$ for 80 LBS
 18 particles, which are almost identical for $l > 1$.

19 Previously, we defined two rotation-invariant SH factors, i.e., AR_{FDE} and
 20 d_{2-8} / d_1 (Zhao et al., 2017). AR_{FDE} is the characteristic aspect ratio for the
 21 first-degree ellipsoid (FDE). This factor has the dominant influence on particle form,
 22 i.e., aspect ratios. $d_{2-8} / d_1 = \sum_{l=2}^8 d_l / d_1$ compares the MSDs of SH degrees between 2
 23 and 8 to that of SH degree 1. This factor has a great influence on particle roundness.
 24 In this study, finer-scale features are also considered by including another SH factor,

25 d_{9-15} / d_1 , which is calculated as $d_{9-15} / d_1 = \sum_{l=9}^{15} d_l / d_1$.

26

27 3. SH coefficient matrices construction method

1 We propose a simple method to construct SH coefficient matrices using four SH
 2 factors, namely, the two aspect ratios of FDE (i.e., AR_{FDE} and EI_{FDE}), d_{2-8}/d_1 , and
 3 d_{9-15}/d_1 . SH coefficient matrices are constructed in two steps. First, an FDE with a
 4 major principal dimension of unit length and specified aspect ratios is generated.
 5 Second, the coefficient matrices of SH degrees between 2 and 8 (i.e., $C_2 - C_8$) and
 6 those between 9 and 15 (i.e., $C_9 - C_{15}$) are constructed from the value of d_{2-8}/d_1
 7 and d_{9-15}/d_1 , respectively.

8 Step-1: First-degree ellipsoid (FDE) with specified EI_{FDE} and FI_{FDE} values (C_1)

9 The shape of an FDE is uniquely determined by its EI and FI values and a unit
 10 major principal dimension. Its principal dimensions ($p_1 \geq p_2 \geq p_3$) are $p_1 = 1$, $p_2 = EI$
 11 and $p_3 = EI \times FI$. Then, FDE's coefficient matrix, C_1 , is constructed as

12
$$-\sqrt{\frac{\pi}{6}} \begin{pmatrix} -1 & 0 & 1 \\ EI \times i & 0 & EI \times i \\ 0 & \sqrt{2}EI \times FI & 0 \end{pmatrix}$$
, where i is the imaginary unit. The generated

13 FDEs have three principal dimensions, p_1 , p_2 , and p_3 , corresponding to x -, y - and
 14 z -axes, respectively.

15 Step-2: Coefficients of SH degrees between 2 and 15 ($C_2 - C_8$ and $C_9 - C_{15}$) with
 16 specified values of d_{2-8}/d_1 and d_{9-15}/d_1

17 The values of d_l for l between 2 and 8 are determined from the specified value of
 18 d_{2-8}/d_1 according to Eq. (5) and the value of d_1 defined in Step-1. Then, we
 19 assume the spherical descriptors have the equivalent decompositions at three
 20 coordination axes, i.e., $d_{x,l} = d_{y,l} = d_{z,l}$. This assumption will balance the decompositions
 21 of MSD on three coordination axes. Therefore, the coefficients of $l > 1$ have limited
 22 influence on particle form.

23 The SH coefficients of C_l are complex numbers that have to satisfy
 24 $c_n^{-m} = (-1)^m c_n^{m*}$ to make the coordinates of vertices to be real numbers. To satisfy this

1 requirement, the form of \mathbf{C}_l is assumed as

$$\begin{aligned}
 \mathbf{C}_l &= \begin{pmatrix} c_{x,l}^{-l} & L & c_{x,l}^0 & L & c_{x,l}^l \\ c_{y,l}^{-l} & L & c_{y,l}^0 & L & c_{y,l}^l \\ c_{z,l}^{-l} & L & c_{z,l}^0 & L & c_{z,l}^l \end{pmatrix} \\
 &= \begin{pmatrix} k_x(\alpha_{2l} - \alpha_{2l+1}i) & L & k_x\alpha_1 & L & k_x(\alpha_{2l} + \alpha_{2l+1}i) \\ k_y(\beta_{2l} - \beta_{2l+1}i) & L & k_y\beta_1 & L & k_y(\beta_{2l} + \beta_{2l+1}i) \\ k_z(\varepsilon_{2l} - \varepsilon_{2l+1}i) & L & k_z\varepsilon_1 & L & k_z(\varepsilon_{2l} + \varepsilon_{2l+1}i) \end{pmatrix}, \tag{6}
 \end{aligned}$$

2
3 where $(\alpha_i, \beta_i, \varepsilon_i)$ for $i \in [1, 2l+1]$ are real numbers between 0 and 1, which are
4 randomly generated with a uniform distribution. k_x , k_y and k_z are three normalizing
5 factors. The values of k_x , k_y and k_z are determined from the values of $d_{x,l}$, $d_{y,l}$ and $d_{z,l}$,

6 e.g., $k_x = \sqrt{d_{x,l}^2 / (\alpha_1^2 + 2 \sum_{i=2}^{2l+1} \alpha_i^2)}$. This procedure is repeated for SH degrees between 2

7 and 8. So far, the coefficient matrices for SH degrees between 2 and 8 are constructed
8 from one specified value of d_{2-8}/d_1 . Similarly, the coefficient matrices of SH
9 degrees between 9 and 15 are determined from d_{9-15}/d_1 .

10

11 **4. Particle shape generation results**

12 In this section, SH coefficient matrices are constructed with a series of SH factors.
13 Then, 3D particle shapes were reconstructed from SH matrices through Eq. 2. The
14 SPHARM-MAT Toolbox is used to perform SH expansion and represent particle
15 shapes with triangular surface meshes for visualization and shape quantification
16 (available at <http://www.iu.edu/~shenlab/software.html>).

17 We first randomly generated three particles from the spherical descriptors of a real
18 LBS particle for SH degrees between 2 and 15. The FDEs for these particles are all
19 unit diameter spheres. Fig. 3 shows the expansions of particles with one or more
20 degrees of SHs superimposing on their FDEs. It shows that higher SH degree
21 describes finer-scale particle features. For example, SH degrees 2 and 4 describe
22 particle roundness, while SH degree 10 describes particle roughness. The overall
23 particle features are well characterized with SH degrees up to 8. The three particles
24 also reflect the randomness of this particle generation method. They have a similar
25 level of irregularity with the original LBS particle but distinct shapes.

26 A series of AR_{FDE} (E_{FDE}) and d_{2-8}/d_1 are used to generate particles with different

1 level of irregularity (Fig. 4). AR_{FDE} (EI_{FDE}) has a dominant influence on particle form.
 2 Particles with large AR_{FDE} (EI_{FDE}) values have almost identical principal dimensions.
 3 As AR_{FDE} (EI_{FDE}) reduces, particles become more elongated. By increasing d_{2-8}/d_1 ,
 4 particles' angularity gradually increases from well rounded to very angular. An
 5 example of well-rounded and angular particle could be pebble and rock ballast,
 6 respectively. Fig.5 shows three particles with different values of d_{9-15}/d_1 , while AR_{FDE}
 7 (EI_{FDE}) and d_{2-8}/d_1 are set as 0.9 (0.9) and zero. It shows that d_{9-15}/d_1 changes particle
 8 roughness without affecting the overall shape.

9 The influence of SH factors on generated particle shapes are quantitatively
 10 investigated using alternate combinations of AR_{FDE} (EI_{FDE}) = {0.5 (0.3); 0.6 (0.5); 0.7
 11 (0.6); 0.8 (0.7); 0.9 (0.9)} and d_{2-8}/d_1 = {0.0; 0.1; 0.2; 0.3; 0.4; 0.5; 0.6} while keeping
 12 d_{9-15}/d_1 equal to zero. For each combination of AR_{FDE} (EI_{FDE}) and d_{2-8}/d_1 , we randomly
 13 generated two hundred particles. Their triangular surface meshes are then quantified
 14 at form, roundness and compactness. Fig.6 plots the average values of the shape
 15 parameters of two hundred particles in each group. It shows that particle form (AR)
 16 and roundness (R_M) are mainly influenced by AR_{FDE} (EI_{FDE}) and d_{2-8}/d_1 , respectively.
 17 Compactness (S and C_X) is influenced by both AR_{FDE} (EI_{FDE}) and d_{2-8}/d_1 . Similarly,
 18 two hundred particles are randomly generated for alternate combinations of AR_{FDE}
 19 (EI_{FDE}) = {0.5 (0.3); 0.6 (0.5); 0.7 (0.6); 0.8 (0.7); 0.9 (0.9)} and d_{9-15}/d_1 = {0.0; 0.01;
 20 0.02; 0.03; 0.04; 0.05; 0.06} while keeping d_{2-8}/d_1 equal to zero. Fig.7 shows that
 21 d_{9-15}/d_1 has a much smaller influence on particle shape parameters than d_{2-8}/d_1 . Only
 22 when AR_{FDE} (EI_{FDE}) is large, particle roundness is slightly influenced by d_{9-15}/d_1 .

23 The two hundred particles in each group generated with the same SH factors have
 24 similar level of irregularity but different shapes. To illustrate this, we picked seven
 25 groups of particles corresponding to the red points in Fig.6. Fig.8 plots the
 26 distributions of their shape parameters. The distributions with enough data points are
 27 fitted with Gaussian function with an offset. The two hundred particles with d_{2-8}/d_1
 28 equal to zero have the same shape parameters. They are identical ellipsoids with the
 29 same AR_{FDE} (EI_{FDE}) and a unit major principal dimension. The randomness of
 30 generated shapes is only introduced by d_{2-8}/d_1 and d_{9-15}/d_1 . The variance of all shape
 31 parameters increases with increasing d_{2-8}/d_1 .

32

33 5. Discussion and summary

34 We proposed a simple method to randomly generate 3D particle shapes with a

1 specified level of irregularity. The SH factors used to generate particle shapes are well
2 correlated with the classical particle parameters. The method has a solid mathematical
3 foundation, i.e., rotation-invariant SH analysis. Therefore, it has great efficiency in
4 calculation and storage cost. For example, generating the SH coefficients (C_1 - C_{15}) of
5 one thousand particles only need 3.70 seconds with an Intel i5-4590 CPU (4 cores, 3.3
6 GHz). These coefficients can be stored in a MAT-file of 5.8 MB. In comparison,
7 generating ten particles takes more than four hours with the discrete random field
8 method proposed in Mollon and Zhao (2014) using the same computer. The MAT-file
9 storing the shape matrix is about 100 MB. Also, the SH descriptors used for particle
10 generation have a strong relationship with classical particle shape parameters. This
11 relationship could serve as an input for generating particles with required shape
12 parameters. The particles generated by this method tend to be smooth due to the
13 nature of SH method. Therefore, it is costly to simulate sharp corners that are
14 common in particle fragments and materials formed via crystallization. It is noticed
15 that further study is needed to understand the influence of the empirical correlation in
16 Eq. (5) on the generated particle shapes.

17 It remains a challenge to quantitatively correlate the micro- and macro-mechanical
18 behaviour of granular assemblies with particle shape. The difficulties mainly arise
19 from the multi-scale nature of particle shape. Also, real particles always have distinct
20 shapes even though they have similar irregularity. For example, no two pebbles are
21 exactly alike, although they are well rounded. The method proposed in this study has
22 great potential for future numerical and experimental studies (e.g. discrete element
23 method and 3D printer) on particle shape. The generated particle shapes have similar
24 irregularity but remains different. This randomness of particle shapes could lead to the
25 a certain level of randomness into the micro- and macro-mechanical behaviour of
26 granular assemblies. However, they should have similar micro- and macro-mechanical
27 behaviours if the behaviours are well correlated with shape irregularity. In addition, a
28 single particle shape could be used to eliminate this randomness.

29

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1 of Tongji University.

2

3 **Notation list**

4	AR	aspect ratio index
5	AR_{FDE}	aspect ratio index of first-degree ellipsoid
6	\mathbf{C}_l	spherical harmonic coefficients matrix of SH degree l
7	$c_{x,l}^m, c_{y,l}^m, c_{z,l}^m$	spherical harmonic coefficient for degree l and order m
8		corresponding to x, y and z coordinates
9	C_X	convexity
10	d_l	spherical descriptor of SH degree l
11	$d_{x,l}, d_{y,l}$ and $d_{z,l}$	three components of d_l corresponding to x, y and z coordinates
12	$e_{l,1} \geq e_{l,2} \geq e_{l,3}$	three eigenvalues of $\mathbf{C}_l \mathbf{C}_l^*$
13	EL_{FDE}	elongation index of first-degree ellipsoid
14	EL	elongation index
15	FDE	first-degree ellipsoid
16	FI	flatness index
17	$p_1 \geq p_2 \geq p_3$	three principal dimensions of FDE
18	R_M	roundness index based on local mean curvature
19	S	sphericity
20	SA	surface area
21	V	volume
22	V_{CH}	volume of convex hull
23	$\mathbf{v}_{\theta,\phi}$	Cartesian coordinates vector
24	Y_l^m	spherical harmonic function for degree l and order m

25

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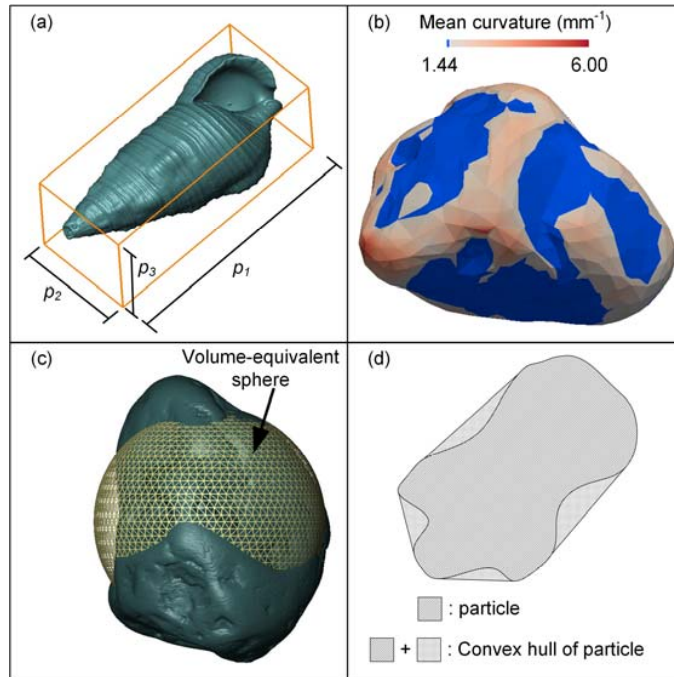


Fig. 1 Illustration of shape parameters: (a) aspect ratios ($El=p_2/p_1$, $Fl=p_3/p_2$, $AR=(El+Fl)/2$); (b) mean-curvature roundness index (R_M); (c) sphericity (S); (d) convexity (C_X).

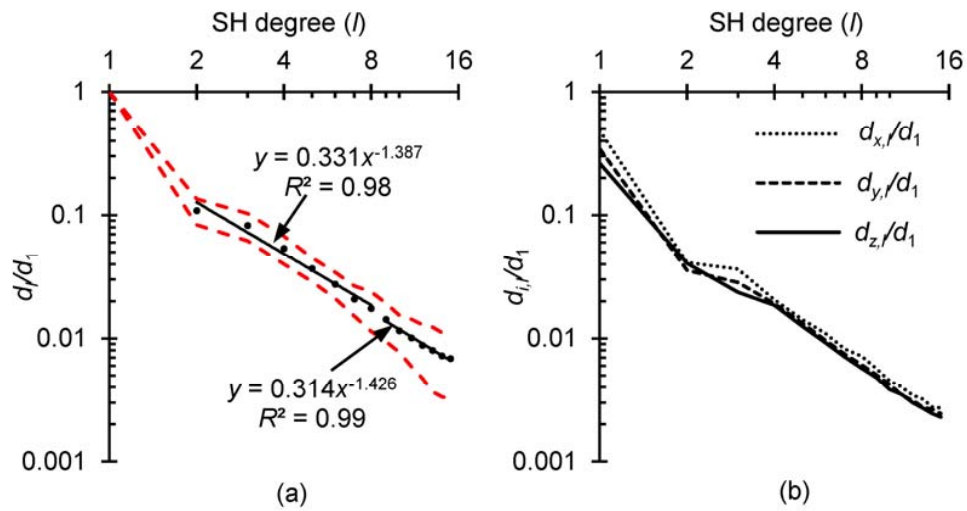


Fig. 2 Spherical descriptors of 80 LBS particles: (a) spherical descriptors at each SH degree (solid lines: mean value; dashed lines: mean value \pm standard deviation) and (b) mean values of spherical descriptors decompositions at x, y and z axes

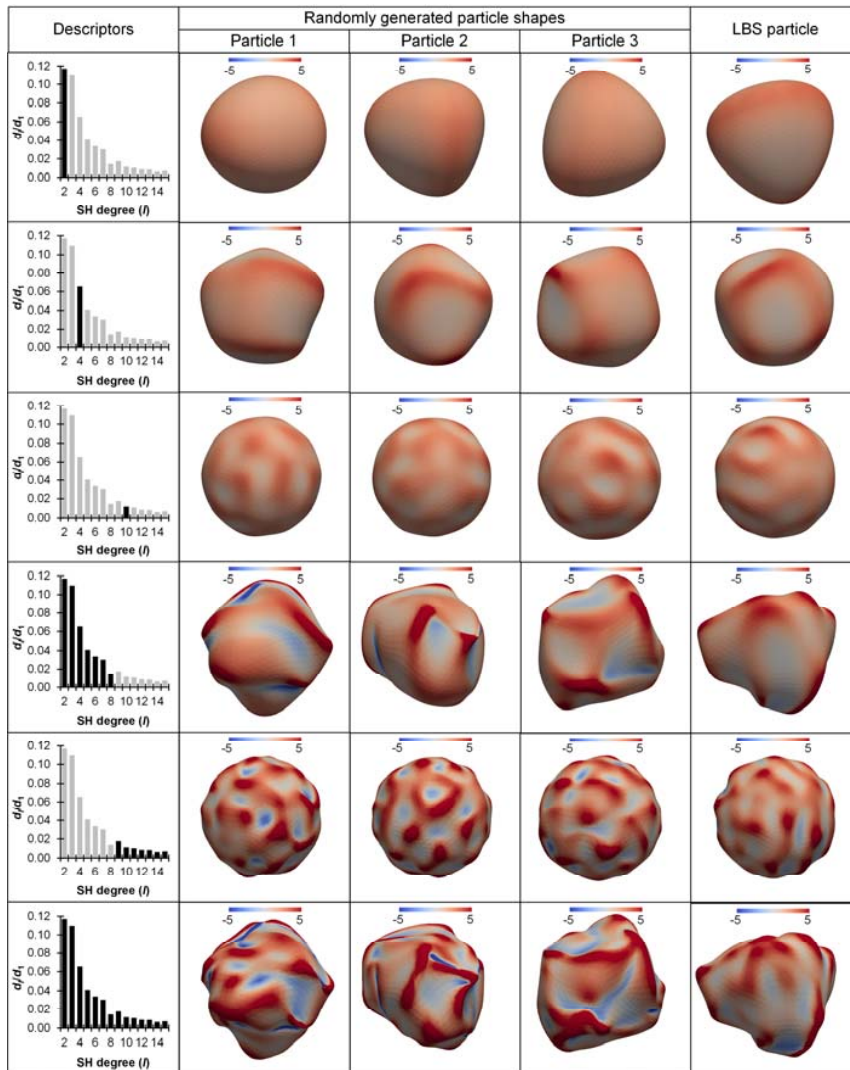


Fig. 3 Three randomly generated particles and a real LBS particle with the same spherical descriptors (d_2 - d_{15}) superimposed on a unit diameter sphere, different SH degrees are used to reconstruct the surfaces (colour of surfaces indicates the distribution of mean curvature, L^{-1})

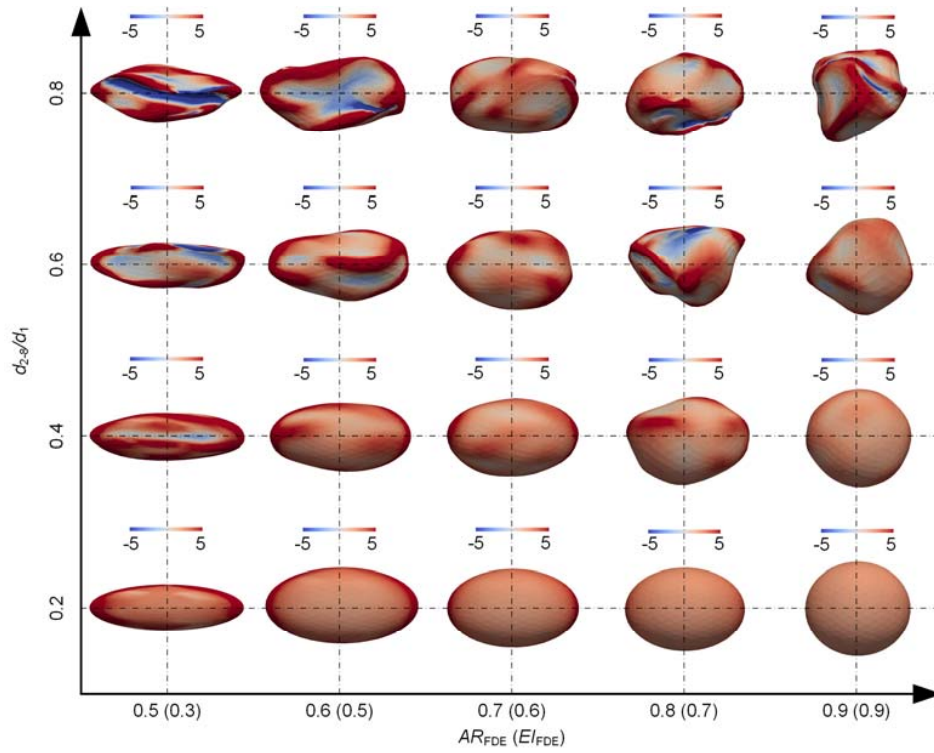


Fig. 4 Influence of $AR_{FDE} (El_{FDE})$ and $d_{2.8}/d_1$ on the shapes of generated particles (colour of surfaces indicates the distribution of mean curvature, L^{-1})

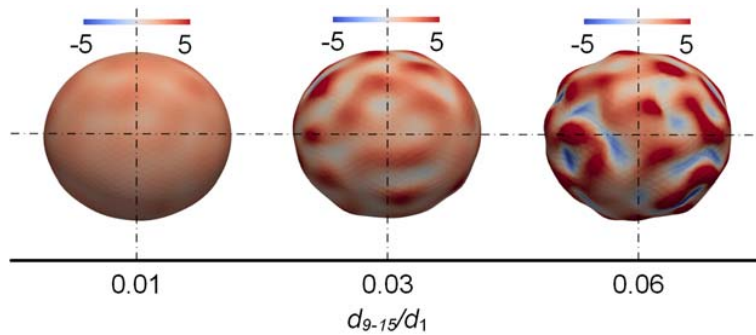


Fig. 5 Influence of $d_{9.15}/d_1$ on the shapes of generated particles (colour of surfaces indicates the distribution of mean curvature, L^{-1})

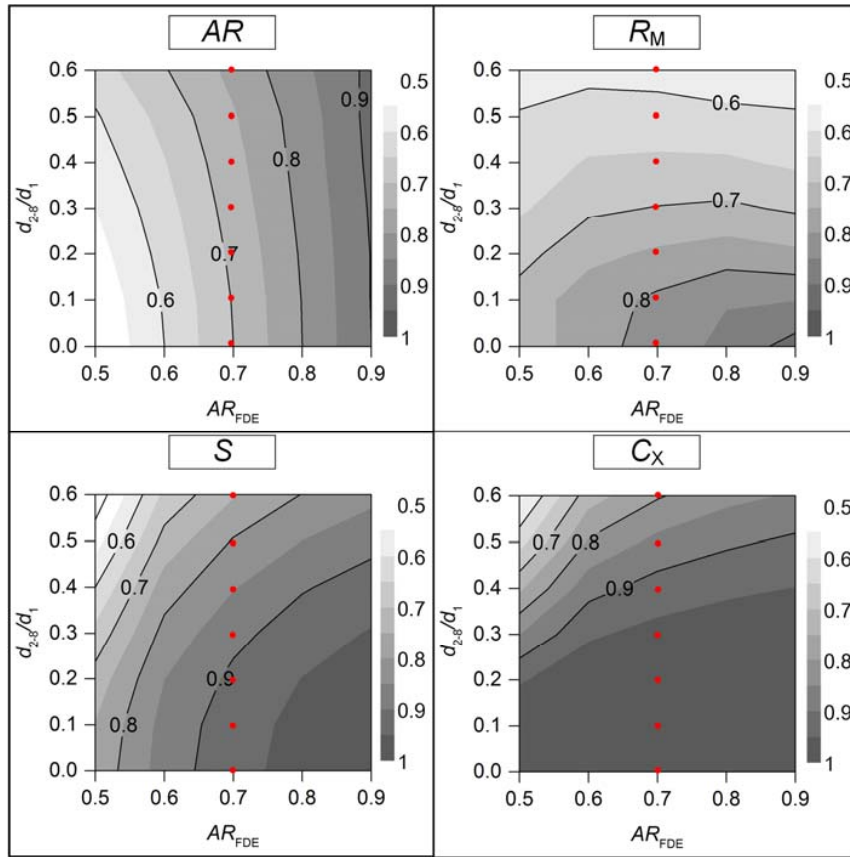


Fig. 6 Mean values of shape parameters (AR , R_M , S and C_X) of 200 randomly generated particles in each combination of AR_{FDE} (EI_{FDE}) = $\{0.5 (0.3); 0.6 (0.5); 0.7 (0.6); 0.8 (0.7); 0.9 (0.9)\}$ and $d_{2-8}/d_1 = \{0.0; 0.1; 0.2; 0.3; 0.4; 0.5; 0.6\}$, while $d_{9-15}/d_1 = \{0.0\}$

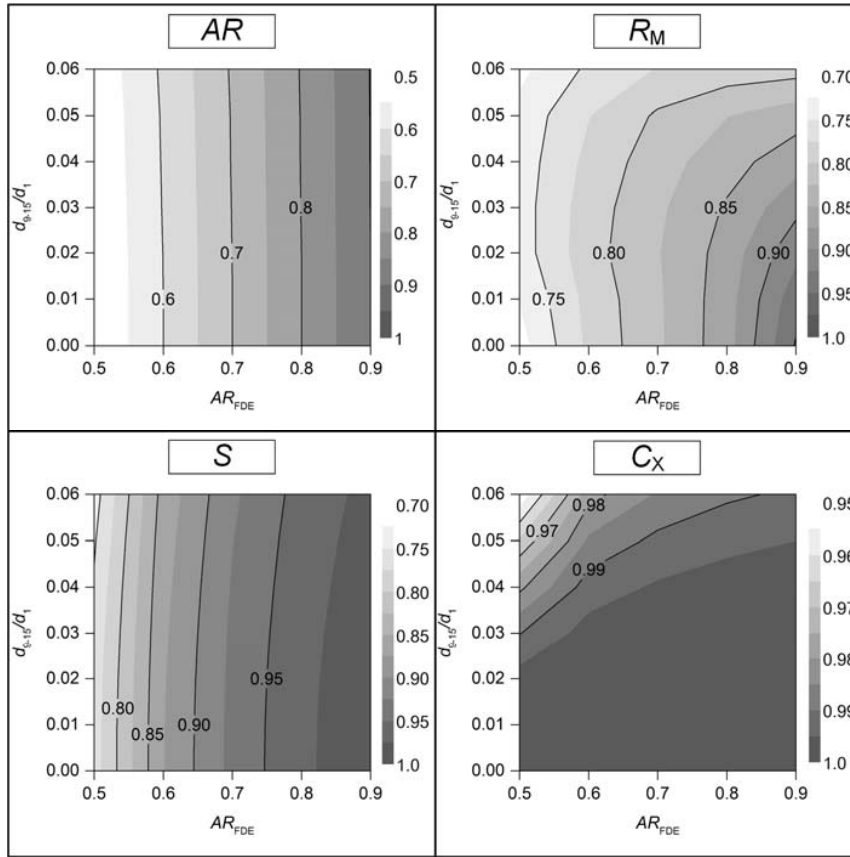


Fig. 7 Mean values of shape parameters (AR , R_M , S and C_X) of 200 randomly generated particles in each combination of AR_{FDE} (EI_{FDE}) = {0.5 (0.3); 0.6 (0.5); 0.7 (0.6); 0.8 (0.7); 0.9 (0.9)} and d_{9-15}/d_1 = {0.0; 0.01; 0.02; 0.03; 0.04; 0.05; 0.06}, while d_{2-8}/d_1 = {0.0}

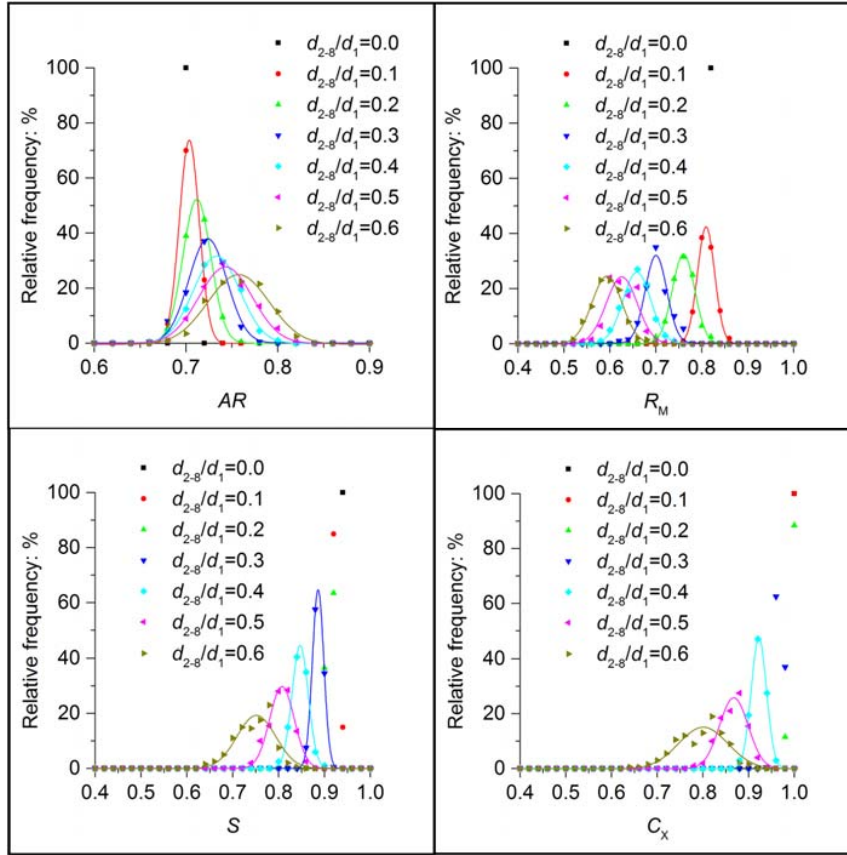


Fig. 8 Distributions of shape parameters (AR , R_M , S and C_x) of 200 randomly generated particles in combinations of AR_{FDE} (EF_{FDE}) = {0.7 (0.6)}, d_{2-8}/d_1 = {0.0; 0.1; 0.2; 0.3; 0.4; 0.5; 0.6} and d_{9-15}/d_1 = {0.0} (distributions with enough data points are fitted with Gaussian function) (corresponding to the red points in Fig.6)