1   # A spherical-harmonic-based approach to discrete element modeling of 3D

2   # irregular particles

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26   **Abstract:** Different from previous discrete element methods (DEM) where irregular 3D

27   particle shapes are approximated by subspheres, vertices or voxels, this study aims to develop

28   an innovative and computationally effective DEM method directly employing spherical

29   harmonic functions for simulations of 3D irregular-shaped particles. First, the discrete surface

30   points of a 3D irregular-shaped particle are represented by spherical harmonic functions with

31   only a limited number of harmonic coefficients to restore the particle morphology. Then, the

32   intrinsic physical quantities are computed directly using spherical harmonic functions. Next,

33   specific algorithms for interparticle overlapping detection and contact resolution involving the

34   spherical harmonic functions are developed. Subsequently, the interparticle contact forces,

35   moments, and particle movements are computed. The feasibility and capability of the proposed

36   3D method is verified by simulating random deposition of superellipsoids, repose angle tests

37   and triaxial tests on particles with various shapes. The proposed method could pave a viable

38   pathway for realistic modeling of granular media pertaining to various engineering and

39   industrial processes.

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1 Introduction

Granular materials, such as sands, gravels and rock aggregates, comprise of particles with various irregular shapes that to a large extent determine the materials' complicated mechanical behaviors and properties [1]-[6]. Different DEM approaches were developed to consider various levels of particle shapes. For instance, for form-scale shape features, ellipses [7], ellipsoids [8][9], elongated particle models with rounded caps [10][11], and spherocylindrical particle models [12] were developed to consider the elongation effects of particles in DEM. Considering the roundness-scale shape features of realistic granular materials, superellipsoid [13], super-quadric [14], egg-shaped particles [15], polyellipsoid [16], and polysuperellipsoid [17] were developed to simulate symmetric and asymmetric shape particles with different corner sharpness. To capture the random irregularities of the granular particles, the polygon/polyhedron-based DEMs were developed by many researchers [18]-**Error! Reference source not found.**. For instance, Feng and Tan [19] used Minkowski-difference to model convex polygon/polyhedron particles. Their proposed method was very effective and also energy-conserving. The Minkowski difference and GJK algorithms have also been implemented for convex polyhedrons in an open-source code SudoDEM [20]. However, these DEMs can hardly replicate the concave and convex surface morphologies of realistic irregular-shaped particles.

To simulate concave and convex irregular-shaped particles, the clump-based DEM was first developed based on the ODEC algorithm [21][22]. Although the clump method enables the investigation of particle-shape effects on various behaviour of particle systems [23][24], the

64   unrealistic multiple contacts between clump-based particles could result in unreasonable

65   simulation results [25]-[27], e.g., over-stiff and over-damped responses. Moreover, some other

66   alternative DEM programs to improve the weakness of clump-based DEM were also proposed,

67   e.g., the granular element method (GEM) [28], the improved NURBS-based DEM [29], the

68   LS-DEM [30]. Nevertheless, when dealing with particles with distinctive sizes and huge

69   numbers, these methods would be computationally expensive.

70   To overcome the abovementioned problems, Lai et al. [31] first developed the FS-DEM to

71   simulate 2D irregular-shaped particles. In the FS-DEM, the arbitrary 2D particle outlines can

72   be continuously described using the Fourier series. However, their study was constrained in 2D

73   plane. There are very limited studies on exploring the possibility of incorporating the harmonic

74   series into DEM to simulate 3D irregular-shaped particles [2][6]. Furthermore, Feng et al.

75   established a generic contact theory for arbitrary shaped particles [32]. Recently, more advanced

76   algorithms were proposed by Feng [33][34] to ensure that the energy is conserved for elastic

77   impact, leading to robust simulations of real problems involving arbitrarily shaped particles.

78   Some successful implementations in both FDEM [35]-[38] and DEM [39][40] have also been

79   conducted to resolve the explicit dynamics of irregular and real shape particles. Overall, it

80   remains a challenge to model arbitrary shapes of realistic particles in DEM.

81   Accordingly, in this study, spherical harmonics, as a well-known higher-dimensional analogy

82   of the Fourier-series, is employed to develop an innovative spherical harmonics-based discrete

83   element method (SH-DEM) for simulating 3D irregular-shaped particles. First, the discrete

84   surface points of a 3D irregular-shaped particle are represented by the spherical harmonic

85   function, where only a limited number of harmonic coefficients are required to restore the

86   particle morphology. Then, the intrinsic physical quantities, which are necessary for

87   computational mechanics, are computed directly using the spherical harmonic function. Next,

88   specific algorithms for overlapping detection and contact resolution are developed for SH-based

89   particles. Subsequently, the computation of the interparticle contact forces, moments, and

90   particle movements is implemented. Finally, several numerical simulations are performed to

91   illustrate the feasibility and capability of the proposed SH-DEM.

2 SH-based irregular-shaped particle model in DEM

2.1 Spherical-harmonic-transform of the particle surface

94   Several advanced techniques, such as X-ray tomography [1] and 3D laser scanning [6], have

95   been employed to acquire the 3D surface information for realistic particles. Since the early

96   2000s, researchers have started to implement the acquisition and modelling of particle systems

97   with real shapes [41]. As illustrated in Fig. 1 (*a*), the obtained 3D surface data is commonly in

98   the format of triangular meshes, which is a typical discretized 3D surface model. As illustrated

99   in Fig. 1 (*b*), the discrete vertices coordinate of the triangular mesh model determines the

100 morphology of the irregular-shaped particle. In order to implement spherical harmonic

101 transformation, the geometrical center of the particle is set as the origin of the spherical

102 coordinate system and the coordination transformation process is performed to transform all

103 the discrete vertices (x, y, z) of triangular meshes into spherical coordinates (θ, φ, r). Once

104 the spherical coordinates of a particle are obtained, the spherical harmonic function can then be

105 used to process the data. The spherical harmonic function is a well-known higher-dimensional

106 analogy of Fourier series, defined on the surface of a sphere. Based on the spherical harmonic

107 function, the surface coordinates $r(\theta, \varphi)$ of a particle can be expressed as the superimposition

108 of a series of spherical harmonic basis functions:

$$r(\theta, \varphi) = \sum_{n=0}^{N} \sum_{m=-n}^{n} a_n^m Y_n^m(\theta, \varphi) \tag{1}$$

109 where N is the highest order number of the spherical harmonic basis functions; $\theta \in [0, \pi]$

110 and $\varphi \in [0, 2\pi]$; $Y_n^m(\theta, \varphi)$ represents the harmonic basis function of order n and degree m;

111 a_n^m is the coefficient corresponding to $Y_n^m(\theta, \varphi)$. A group of N harmonics contains

112 $(N + 1)^2$ number of a_n^m and $Y_n^m(\theta, \varphi)$. The basic function $Y_n^m(\theta, \varphi)$ is defined as:

$$Y_n^m(\theta, \varphi) = \sqrt{\frac{(2n + 1)(n - |m|)!}{4\pi(n + |m|)!}} P_n^m(\cos \theta) e^{im\varphi} \tag{2}$$

113 where $P_n^m(x)$ is the related Legendre polynomial:

$$P_n^m(x) = (-1)^{|m|} \cdot (1 - x^2)^{\frac{|m|}{2}} \cdot \frac{d^{|m|} P_n(x)}{dx^{|m|}} \tag{3}$$

114 in which $P_n(x)$ is the nth order Legendre polynomial:

$$P_n(x) = \frac{1}{2^n n!} \frac{d^n[(x^2 - 1)^n]}{dx^n} \tag{4}$$

115 Assume that there are a total of N_P points on the particle surface. Substituting these N_P

116 spherical coordinates $r(\theta, \varphi)$ into Eq. (4), we can obtain N_P linear equations:

$$
\begin{cases}
r_1 = \sum_{n=0}^{N} \sum_{m=-n}^{n} a_n^m Y_n^m(\theta_1, \varphi_1) \\
\qquad \vdots \\
r_i = \sum_{n=0}^{N} \sum_{m=-n}^{n} a_n^m Y_n^m(\theta_i, \varphi_i) \\
\qquad \vdots \\
r_{N_P} = \sum_{n=0}^{N} \sum_{m=-n}^{n} a_n^m Y_n^m(\theta_{N_P}, \varphi_{N_P})
\end{cases}
\tag{5}
$$

117   In Eq. (5), $r_1 \sim r_{N_P}$ and $Y_n^m(\theta_1, \varphi_1) \sim Y_n^m(\theta_{N_P}, \varphi_{N_P})$ are all known while there are

118    $(N+1)^2$ unknown coefficients a_n^m. It is worth noting that, according to the previous studies

119   [1], N = 15 is probably sufficient to represent the particle morphology. Since N_P can always

120   be much larger than $(N+1)^2$, it is easy to solve these coefficients with N_P equations through

121   least-squares estimation.

122   **2.2 Representation of particle surface by inverse SHT**

123   After $(N+1)^2$ harmonic coefficients are obtained for the discrete surface points of a target

124   particle, as detailed in Section 2.1, we can use the $(N+1)^2$ harmonic functions to represent

125   the discretized surface points as a continuous closed surface. This process, namely the inverse

126   operation of spherical harmonic transformation, is described as follows:

127   (1) Assume a random point $P_i(r_i, \theta_i, \varphi_i)$ with polar radius r_i and polar angle (θ_i, φ_i) is on

128   the particle surface. When N_P surface points are required, N_P unit vertices

129    $[(1, \theta_1, \varphi_1), \cdots, (1, \theta_i, \varphi_i), \cdots, (1, \theta_{N_P}, \varphi_{N_P})]$ uniformly surrounding the origin of the spherical

130   coordinate system is determined based on the antipodal symmetry based scheme as adopted in

131   the our previous work [3]. These unit vertices can be regarded as a series of points equally

132   distributed on a sphere. Then, based on the spherical harmonic function, compute the

133   corresponding surface points $\left[(1, \theta_1, \varphi_1), \cdots, (1, \theta_i, \varphi_i), \cdots, \left(1, \theta_{N_P}, \varphi_{N_P}\right)\right]$ on the particle. It

134   should be noted that N_P needs to be sufficiently large if a high-quality 3D triangular mesh

135   model is required.

136   (2) Substitute (θ_i, φ_i) into Eq. (3) to obtain the corresponding $Y_n^m(\theta_i, \varphi_i)$. For a certain

137   harmonic order n, superimpose $(2n + 1)$ $a_n^m Y_n^m(\theta, \varphi)$ together, where m is the integer

138   varying from $-n$ to n. Repeat this process from $n = 1$ to N, and superimpose them to obtain

139   the final result of $r(\theta, \varphi)$.

140   (3) Finally, the coordinate transform can be used to obtain the Cartesian coordinates (x_i, y_i, z_i)

141   of the particle surface. Fig. 1 (*c*) illustrated the reconstructed SH-based model. Since the above-

142   detailed inverse SHT process can be used to calculate the coordinates of any surface points P_i,

143   the 3D irregular-shaped particle surface can thus be continuously represented by the spherical

144   harmonic function.

145   **2.3 Intrinsic physical quantities of SH-based particle**

146   The intrinsic physical quantities, such as the mass and moment of inertia, for each SH-based

147   particle, can be directly calculated from the adopted spherical harmonic functions that are used

148   to generate the corresponding particle.

149   (1) Mass of a 3D irregular-shaped particle

150   The mass of a 3D irregular-shaped particle with uniform density ρ can be computed by:

$$m = \rho \cdot V \tag{6}$$

151   where V is the volume of the SH-based particle. In the proposed SH-DEM approach, the

152   volume of the particle can be calculated by integrating the radical distance r over the spherical

153   angles θ, φ:

$$V = \frac{1}{3} \int_0^\pi \int_0^{2\pi} r(\theta, \varphi)^3 \sin(\theta) d\varphi \, d\theta \tag{7}$$

154   where the radical distance r at any spherical angle pair (θ, φ) can be obtained using the

155   spherical harmonic function, as given in Eq. (1).

156   (2) Moment of inertia

157   For an SH-based particle, the moment of inertia around three Cartesian coordinate axes can be

158   expressed as a tensor $\boldsymbol{I}$:

$$\boldsymbol{I} = \begin{bmatrix} I_{xx} & -I_{xy} & -I_{xz} \\ -I_{xy} & I_{yy} & -I_{yz} \\ -I_{xz} & -I_{yz} & I_{zz} \end{bmatrix} \tag{8}$$

159   where I_{xx}, I_{xy}, I_{yz}, I_{yy}, I_{xz} and I_{zz} can be calculated by:

$$I_{xx} = \frac{1}{5} \rho \int_0^\pi \int_0^{2\pi} r(\theta, \varphi)^5 \sin(\theta) \left((\sin(\theta) \sin(\varphi))^2 + (\cos(\theta))^2 \right) d\varphi d\theta$$

$$\tag{9}$$

$$I_{yy} = \frac{1}{5} \rho \int_0^\pi \int_0^{2\pi} r(\theta, \varphi)^5 \sin(\theta) \left((\sin(\theta) \cos(\varphi))^2 + (\cos(\theta))^2 \right) d\varphi d\theta$$

$$I_{zz} = \frac{1}{5}\rho \int\limits_0^\pi \int\limits_0^{2\pi} r(\theta,\varphi)^5 \sin(\theta)^3 \, d\varphi d\theta$$

$$I_{xy} = \frac{1}{5}\rho \int\limits_0^\pi \int\limits_0^{2\pi} r(\theta,\varphi)^5 \sin(\theta)^3 \cos(\varphi)\sin(\varphi) \, d\varphi d\theta$$

$$I_{xz} = \frac{1}{5}\rho \int\limits_0^\pi \int\limits_0^{2\pi} r(\theta,\varphi)^5 \sin(\theta)^2 \cos(\theta) \cos(\varphi) \, d\varphi d\theta$$

$$I_{yz} = \frac{1}{5}\rho \int\limits_0^\pi \int\limits_0^{2\pi} r(\theta,\varphi)^5 \sin(\theta)^2 \cos(\theta)\sin(\varphi) \, d\varphi d\theta$$

160   It is worth noting that, the tensor I needs to be computed first based on a coordinate system

161   (whatever it is), then the principal moment axes are obtained to form a local coordinate system.

162   Finally, the SH-based particles will always be rotated at the local frame where each principal

163   moment of inertia is along one coordinate axis.

3 Computation of interactions between SH-based particles

165   In this section, we develop unique algorithms for overlapping detection and contact resolution

166   of SH-based particles. First, the spherical harmonic function is combined with the node-to-

167   surface approach to examine the overlapping condition between two collision candidate

168   particles. Second, the contact point and contact normal vector of each penetration node can be

169   quickly calculated based on the proposed scheme in the SH-DEM. Third, the normal contact

170   force is computed for each penetration node based on the volumetric normal contact stiffness

171   and local overlapping volume.

172   **3.1 Overlapping detection for 3D irregular-shaped particle**

173   (1) Global overlapping detection

174   In the first stage, irregular-shaped particles are circumscribed by the axis-aligned bounding

175   boxes (AABBs). The boundaries $(X_{min}, X_{max}, Y_{min}, Y_{max}, Z_{min}, Z_{max})$ of the AABB for a 3D

176   irregular-shaped particle are illustrated in Fig. 2. Then, the modeling domain is divided into

177     $N_{bx} \times N_{by} \times N_{bz}$ cubic bins. Next, the obtained AABBs are entered into cells (i.e., spatial bins)

178   in the cell space based on an enlarged extent (i.e., cell extent). Once the cell extents of two

179   particles overlap, the two particles are considered as a collision candidate. More specifically, if

180   a particle shares at least one single cell bin with one of its neighbors, further detection is

181   required to examine the potential collision between them.

182   (2) Local overlapping detection

183   The spherical harmonic function is combined with the node-to-surface approach to examine the

184   local overlapping condition if two neighboring particles are detected as potentially overlapped

185   using the global overlapping detection algorithm. The node-to-surface scheme has previously

186   been employed in finite element methods [42][43] as well as discrete element methods [30][44]

187   to deal with the contact problems between irregular-shaped particles where the contact interface

188   is non-convex shape and multiple contact points may exist. The detailed procedure for the local

189   overlapping detection is as follows:

190   Step 1: If two neighboring particles are detected as potentially overlapping at the global

191   overlapping detection stage, select the particle with a smaller volume as a Master Grain (MG),

192   while the other is regarded as the Slave Grain (SG). Then, as illustrated in Fig. 3, under the local

193   spherical coordination system of the MG (in blue), determine the potential overlapping range

194   (in red) of spherical angles where the circumscribed spheres of the two particles intersect.

195   Step 2: As illustrated in Fig. 4, the SG is represented by the spherical harmonic function

196    $r^S(\theta, \varphi)$, while the particle surface of the MG in the potential overlapping range is discretized

197   into triangular meshes with a certain number of vertices $Q_i[r_i^M(\theta_i, \varphi_i)]$, which are seeded on

198   the particle surface at a uniform interval based on the antipodal symmetry based scheme as

199   adopted in our previous work [3]. It is worth noting that the density of the discretized nodes on

200   the MG can be quantitatively controlled and easily increased if more accurate modeling

201   resolution is required.

202   Step 3: Transform each of the discretized vertices on the MG from its local coordinate system

203   into the local spherical coordinate system of the SG, $Q_i[r_i^M(\theta_i, \varphi_i)]$. Then, as illustrated in Fig.

204   5, the overlapping condition is determined by checking each $Q_i[r_i^M(\theta_i, \varphi_i)]$ against the SH-

205   based surface function $r^S(\theta, \varphi)$ of the SG for penetration. If $Q_i[r_i^M(\theta_i, \varphi_i)] > r^S(\theta_i, \varphi_i)$, the

206   vertex $Q_i[r_i^M(\theta_i, \varphi_i)]$ is outside the surface of the SG. If $Q_i[r_i^M(\theta_i, \varphi_i)] = r^S(\theta_i, \varphi_i)$,

207    $Q_i[r_i^M(\theta_i, \varphi_i)]$ lies on the surface of the SG. If $r_i^M(\theta_i, \varphi_i) < r^S(\theta_i, \varphi_i)$, vertex

208    $Q_i[r_i^M(\theta_i, \varphi_i)]$ penetrates the boundary of the SG. If any of the node Q_i is detected to

209   penetrate the SG, the overlap between MG and SG is then identified. It is noted that the density

210   of the discretized vertices on the potential overlapping region of the MG will not influence the

211   underlying surface morphology of the original particle, which is represented by its spherical

212   harmonic function, but the accuracy and computational cost will be affected.

213   **3.2 Contact resolution for 3D irregular-shaped particle**

214   As mentioned in the previous subsection, if overlapping is identified, the penetrating vertices

215   $Q_i[r_i^M(\theta_i, \varphi_i)]$ of MG with $r_i^M(\theta_i, \varphi_i) < r^S(\theta_i, \varphi_i)$ can be extracted for the computation of

216   contact points and inter-particle forces. For each penetrating vertex $Q_i[r_i^M(\theta_i, \varphi_i)]$ of the MG

217   inside the SG, there is a corresponding vertex $P_i[r^S(\theta_i, \varphi_i)]$ on the SG by directly substituting

218   (θ_i, φ_i) into the spherical harmonic function of $r^S(\theta, \varphi)$ of SG. For each pair of vertices Q_i

219   and P_i, the contact point C_i, contact normal vector $\vec{n}_i$, and local overlapping volume V_i can

220   be defined as follows:

221   (1) Contact point C_i

222   As illustrated in Fig. 6, the midpoint of the penetration points Q_i and P_i is defined as the

223   contact point C_i for the local overlapping region of Q_iP_i, i.e., $C_i = (Q_i + P_i)/2$.

224   (2) Contact normal vector $\vec{n}_i$

225   As illustrated in Fig. 7, the sum of the outward normal vector $\vec{n}_i^Q$ at vertex Q_i on the surface

226   of MG and the inward normal vector $\vec{n}_i^P$ at P_i on the surface of SG are computed to define

227   the contact normal vector $\vec{n}_i$:

$$\vec{n}_i = \frac{\vec{n}_i^Q + \vec{n}_i^P}{\|\vec{n}_i^Q + \vec{n}_i^P\|} \tag{10}$$

228   where $\vec{n}_i^Q$ is the inward normal vector at vertex Q_i on the MG, and $\vec{n}_i^P$ is the outward normal

229   vector at vertex P_i on the SG.

230   The contact normal vector is simple and easy to compute due to the formulation of the spherical

231   harmonic function, whose outward normal vector at any spherical angle (θ, φ) can be easily

232   obtained by:

$$\vec{n}(\theta, \varphi) = \left(-\frac{\partial \vec{R}(\theta, \varphi)}{\partial \theta} \times \frac{\partial \vec{R}(\theta, \varphi)}{\partial \varphi} \right) \tag{11}$$

233   where $\vec{R}(\theta, \varphi)$ is the position vector of the vertex, which is represented in the Cartesian

234   coordinate system as:

$$\vec{R}(\theta, \varphi) = [r(\theta, \varphi) \cos \theta \cos \varphi, \quad r(\theta, \varphi) \cos \theta \sin \varphi, \quad r(\theta, \varphi) \sin \theta] \tag{12}$$

235   (3) Local overlapping volume V_i

236   As illustrated in Fig. 8, the local overlapping volume V_i can be computed by:

$$V_i = \frac{1}{3} \sum V_{P_i P_i^k P_i^{k+1} Q_i Q_i^k Q_i^{k+1}} \tag{13}$$

237   where (Q_i^k, Q_i^{k+1}) is the kth pair of the one-ring neighboring vertex of Q_i on the MG, the

238   definition of one-ring neighboring vertex has been detailed in our previous work [5];

239   (P_i^k, P_i^{k+1}) are the vertices on the SG that correspond to (Q_i^k, Q_i^{k+1}), which can be obtained

240   by directly substituting $(\theta_i^k, \varphi_i^k)$ and $(\theta_i^{k+1}, \varphi_i^{k+1})$ into the spherical harmonic function of

241    $r^S(\theta, \varphi)$ of SG. As shown in Fig. 8 (d), $V_{P_i P_i^k P_i^{k+1} Q_i Q_i^k Q_i^{k+1}}$ is the volume of the polyhedron

242   formed by the six vertices. As shown in Fig. 8 (e), the local overlapping volume V_i is formed

243   by Q_i, P_i, and the midpoints between their one-ring neighboring vertices.

3.3 Force and moment for 3D irregular-shaped particle

Different from the existing clump-based [21] and polyhedral-based [20] DEM, in the proposed

SH-DEM, the contact forces between the identified neighboring particles are computed based

on the defined contact point, normal contact direction, and local overlapping volume at each

penetration node. The volume-based contact model is employed in the proposed SH-DEM to

compute the normal contact force. It is worth noting that, as suggested by Feng [32]-[34], the

conventional volume-based contact models may have a problem of energy increase for an

elastic impact and thus becomes a source of potentially numerical instability. Thus, the energy-

conserving contact theory [32]-[34] will be incorporated into the SHDEM in the future work to

enhance the reliability and accuracy of the simulation.

The normal contact force at the contact point Q_i' resulting from the corresponding SG to MG

is formulated as:

$$\vec{F}^M_{n,i} = k_n V_i' \vec{n}_i'$$

(14)

where k_n is the volumetric normal contact stiffness. If the material properties of the two

touching irregular-shaped particles are different, k_n can be determined by:

$$k_n = \frac{k_n^M k_n^S}{k_n^M + k_n^S}$$

(15)

where the superscripts M and S denote the master grain and slave grain in contact.

By action and reaction, the resulting normal contact force at the contact point C_i' from the

corresponding MG to SG can be computed as:

$$\vec{F}_{n,i}^S = -\vec{F}_{n,i}^M \tag{16}$$

261   Similar to other existing DEM algorithms, the tangential contact force is determined by the

262   Coulomb friction model. To calculate the resultant tangential contact force $\vec{F}_{t,i}^M$ at the contact

263   point C_i' from SG to MG, the relative velocity $\vec{v}_i^M$ of C_i' to the SG is:

$$\vec{v}_i^M = \vec{v}^M + \boldsymbol{\omega}^M \times (\boldsymbol{C}_i' - \boldsymbol{c}^M) - \vec{v}^S - \boldsymbol{\omega}^S \times (\boldsymbol{C}_i' - \boldsymbol{c}^S) \tag{17}$$

264   where $\vec{v}^M$ and $\boldsymbol{\omega}^M$ are the translational and angular velocities of the MG, $\vec{v}^S$ and $\boldsymbol{\omega}^S$ are

265   the translational and angular velocities of the SG, $\boldsymbol{c}^M$ and $\boldsymbol{c}^S$ are the mass centers of the MG

266   and SG, respectively.

267   Then, the incremental tangential displacement Δu of the MG at the contact point C_i' relative

268   to the SG is:

$$\Delta u = [\vec{v}_i^M - (\vec{v}_i^M \vec{n}_i')\vec{n}_i']\Delta t \tag{18}$$

269   Next, the tangential force from the SG on the MG at the contact point C_i' after Δt is updated

270   as:

$$\vec{F}_{t,i}^M = \frac{\boldsymbol{Z}\vec{F}_{t,i}^{M'}}{\left\|\boldsymbol{Z}\vec{F}_{t,i}^{M'}\right\|} \min\left\{\left\|\boldsymbol{Z}\vec{F}_{t,i}^{M'} - k_t\Delta u\right\|, \mu\left\|\vec{F}_{n,i}^M\right\|\right\} \tag{19}$$

271   where $\boldsymbol{Z}$ is the rotation matrix that rotates the normal vector $\vec{n}_i'$ at the current time step to the

272   normal vector at the previous time step, k_t is the tangential contact stiffness, and μ is the

273   inter-particle friction coefficient. The occurrence of slide events at the contact is determined by

274   the sliding friction model. If $\left\|\boldsymbol{Z}\vec{F}_{t,i}^{MS'} - k_t\Delta u\right\|$ is greater than $\mu\left\|\vec{F}_{n,i}^{MS}\right\|$, the slide event occurs

275 at the contact and $\vec{F}_{t,i}^{MS}$ is reduced to $\mu\|\vec{F}_{n,i}^{MS}\|$.

276 By action and reaction, the tangential force from MG on SG at the contact point C_i' is

$$\vec{F}_{t,i}^{S} = -\vec{F}_{t,i}^{M} \tag{20}$$

277 The moment $\overrightarrow{M}_i^{M}$ contributed by the normal and tangential contact force $\vec{F}_{n,i}^{M}$, $\vec{F}_{t,i}^{M}$ at the

278 contact point CP_i^{M}, resulting from the SG to the MG, is formulated by:

$$\overrightarrow{M}_i^{M} = (C_i' - c^M) \times (\vec{F}_{t,i}^{M} + \vec{F}_{n,i}^{M}) \tag{21}$$

279 Similarly, the moment $\overrightarrow{M}_i^{S}$ contributed by the normal and tangential contact force $\vec{F}_{n,i}^{S}$, $\vec{F}_{s,i}^{S}$

280 at the contact point C_i', resulting from the MG to the SG, is formulated by:

$$\overrightarrow{M}_i^{S} = (C_i' - c^S) \times (\vec{F}_{t,i}^{S} + \vec{F}_{n,i}^{S}) \tag{22}$$

281 **3.4 Particle kinematics and computational scheme**

282 To simulate the kinematics of a large number of 3D irregular-shaped particles, the explicit time

283 step approach is employed to compute the motion of the SH-based particles. The law of force-

284 displacement (constitutive contact law) and the law of motion (Newton's second law) are used

285 to calculate the contact force between particles and the movement of each particle at each time

286 step, respectively. The computation of particle kinematics in the SH-DEM is detailed in

287 Appendix A.

288 It is important to note that, to minimize the computational cost, the spherical harmonic function

289 and corresponding discretized vertices of each SH-based particle are never updated as the

290   particle moves; each spherical harmonic function remains in a reference configuration. To

291   accommodate this constraint, when computing the contact, the discretized nodes of the MG are

292   first transformed temporarily from its local spherical coordinate system into the global

293   Cartesian coordinate frame and are subsequently transformed temporarily into the reference

294   configuration of the SG. In the local spherical coordinate system of the SG, the contact forces

295   and moments are computed and then tranformed back to the global coordinate system.

296   The whole computation procedure for irregular-shaped particle kinematics in the SH-DEM,

297   which follows conventional DEM codes, is detailed in Appendix B. The proposed SH-DEM

298   exhibits great efficiency in updating the irregular particle information at each time-step. Since

299   each particle is represented by the spherical harmonic function, it only requires a few variables

300   (i.e., the position of the particle center and the rotation angle of the local particle coordinate

301   with reference to the global specimen coordinate) to restore the irregular 3D particle shapes.

302   The harmonic coefficients remain constant and are independent of the particle motion and

303   kinematics.

304   4 Numerical examples

305   4.1 Random packing of superellipsoid particles

306   Simulating the random packing of aspherical particles, e.g., superellipsoids, has been a hot issue

307   among granular researchers [13][50][51] for many years. Through various laboratory

308   experiments and numerical simulations, it has been revealed by many researchers that

309   elongation and flatness play a significant role in both packing density and microscopic

310   structures of super-ellipsoid particles. Therefore, before simulating realistic irregular-shaped

311   particles, we first focus on the random packing of ellipsoid particles to examine the consistency

312   of SH-DEM simulations with existing studies. In this section, we focus on a typical type of

313   super-ellipsoid particles with various form and blockiness shapes, which are determined by the

314   shape control parameters η and ζ:

$$\left|\frac{x}{\eta c}\right|^{\frac{2}{\zeta}} + \left|\frac{y}{\eta c}\right|^{\frac{2}{\zeta}} + \left|\frac{z}{c}\right|^{\frac{2}{\zeta}} = 1 \tag{23}$$

315   where η determines the form shape, ζ determines the blockiness shape, and c determines

316   the particle size. The adopted shapes generated by Eq. (23) are all special cases of super-

317   quadrics [50][51].

318   In this section, we aim to reproduce the packing features of superellipsoid particles with η

319   varying from 0.4 to 2.5 while ζ varying from 0.5 to 1.5. To ensure that the simulated packing

320   features are only affected by the shape, the other particle properties are set to the same values

321   for all simulation scenarios. The particle size r, defined as the radius of the sphere with

322   equivalent volume) for each particle, is set as 10mm. The DEM simulation parameters are listed

323   in Table 1, which are typical values for the simulation of rock aggregates in previous works

324   [13][45]. To balance the modeling accuracy and the computational cost, N is set to 20 and Np

325   is set to 8000.

326   The gravitational layer-by-layer deposition approach is employed to simulate the random

327   packing of superellipsoid particles. Each sample consists of 1200 non-overlapping particles,

328   i.e., 12 layers of 100 particles are sequentially added to a box. The box used to contain the

329   particles is 100 mm in width and 100 mm in length. The height is set to 150 mm to facilitate

330   enough space to allocate each layer of non-overlapping particles above existing particles. For

331   each layer, 100 particles of 10 mm in diameters with random locations and orientations are

332   distributed without overlapping in the box. When the existing particles reach an assumed

333   equilibrium state, the next layer of particles is added sequentially. Fig. 9 shows some final

334   packings for an initial observational comparison.

335   In the present study, two groups of particle shapes controlled by 12 values of η (Group A) and

336   12 values of ζ (Group B) are simulated to examine the macroscopic property - packing density.

337   The simulation results are detailed as follows:

338   The packing density ρ of a granular particle assembly can be calculated as the volumetric

339   percentage of the solid particles versus the total volume of the particle assembly, including

340   particles and voids. As shown in Fig. 10 (*a*), for group A, the evolution of packing density versus

341   increasing value of η for superellipsoid particles with $\zeta = 1$ are plotted and compared with

342   the existing studies [13][46][47]. It can be seen in the figure that the trend is consistent with the

343   results of other simulation studies in the previous literature. In general, all studies show two

344   peak values of packing density. The first peak value of packing density exists when η is

345   approximately 0.6, and the second peak value of packing density can be observed when η

346   reaches approximately 1.5. This evolution trend of packing density versus η can be described

347   as an "M" shaped relationship. This "M" shaped relationship between packing density and η

348   is obviously observed in both the present and existing simulations. As shown in Fig.10 (*b*), for

349 group B, the evolution of packing density versus increasing value of ζ for superellipsoid

350 particles with $\eta = 1$ are plotted and compared with the existing studies [13][48][49]. It is

351 observed that there is a valley in the ζ-ρ curve, i.e., the particles with $\zeta = 1$ exhibit the lowest

352 packing density. When ζ increases from 0.3 to 1.0, the packing density shows a negative

353 relationship with ζ. When ζ further increases to be larger than 1.0, the packing density

354 becomes positively related to ζ. This "V" shaped trend was also reported in previous

355 simulations [13][48][49].

356 **4.2 Repose angle tests of real crushed rock aggregates**

357 The repose angle is a well-acknowledged physical property that has been employed by many

358 researchers to calibrate the inter-particle friction coefficient of granular materials needed for

359 DEM analysis. In this study, laboratory experiments for measuring the repose angle of crushed

360 rocks are conducted, and the results are used to verify the validity of the developed SH-DEM

361 program. The repose angle tests are conducted inside a container with glass sidewalls and a

362 stone base, whose dimensions are 10 cm in width, 40 cm in length, and 20 cm in height, as

363 shown in Fig. 11 (*a*). The crushed rocks are granite, with average aggregate sizes of 20 mm in

364 diameter. In the test, approximately 300 crushed rocks are poured into the right part of the

365 container, which is supported by a sidewall (baffle) at right, as shown in Fig. 11 (*b*). The

366 dimensions of the rock assembly are kept as 10 cm in width, 10 cm in length, and 20 cm in

367 height. Then, to ensure an optimal spreading of the material, the sidewall is lifted using a small

368 velocity, as shown in Fig. 11 (c). During wall lifting, the crushed rocks collapse, roll and form

369 a slope under gravity. Finally, after the collapsed crushed rocks stabilized, the repose angle is

370   measured using an angular ruler, as illustrated in Fig. 11 (*d*). The tests are repeated 20 times,

371   and the experimental results reveal that the tested crushed rocks have an average repose angle

372   of approximately 38.9°.

373   A numerical analysis of the angle of repose is performed using the proposed SH-DEM. As

374   shown in Fig. 12, the real crushed rocks are first scanned using the 3D laser scanner, and the

375   surface cloud points are imported into the SH-DEM to obtain realistic SH-based rock

376   aggregates. The simulation process follows the same sequence as the laboratory experiment.

377   First, the initial numerical samples for testing are prepared by sequentially adding the randomly

378   selected SH-based real rocks into the right-side container, which consists of four virtual

379   sidewalls in the DEM. At this stage, contact frictions are all set to 0.0 to guarantee a relatively

380   dense packing condition. Other DEM simulation parameters follow previous studies, as listed

381   in Table 1. As shown in Fig. 13 (*a*), the dimension of the initial sample is the same as the real

382   case. During the simulation, the contact friction coefficient between rocks (aggregate to

383   aggregate and aggregate to base-wall) is set to a specific value, and then the simulated baffle

384   (in red) is slowly lifted, as shown in Fig. 13 (*b*). For each value of the contact friction coefficient,

385   the tests are repeated 20 times to compute a mean repose angle, and the contact friction

386   coefficient is incrementally changed to bring the simulated mean repose angle close to the

387   average laboratory-measured value. Fig. 14 illustrates the repose angles of the samples with

388   different contact friction coefficients. The results indicate that the contact friction coefficient

389   should be taken as approximately 0.3 to simulate the realistic repose angle of crushed rocks.

390   The macroscopic and microscopic properties of rock aggregate assemblies are of great

391   importance to assessing engineering behaviors of the geo-body and the construction-body, e.g.,

392   slope, foundation, embankment, etc. Many researchers have reported that there are many factors,

393   e.g., confining pressure, initial void ratio, and aggregate shape can significantly influence on

394   the macro- and micromechanical properties of crushed rocks. In this section, we aim to examine

395   the shape effects on the macro- and micromechanical properties of the rock assemblies during

396   repose angle tests. Three simulations were conducted with crushed rock aggregates of various

397   shapes. Fig. 15 shows the ranges of shapes and the snapshots of example aggregates, where

398   sample S1 consists of spherical aggregates with AR=1.0, sample S2 consists of ellipsoidal

399   aggregates with AR=0.65, and Sample S3 consists of real crushed rocks with mean AR=0.65.

400   In the simulation, the material properties are consistent with the previous section, while the

401   contact friction between rocks is kept as 0.3 during the baffle lifting and rock collapsing stages.

402   The simulation results are detailed as follows:

403   (1) Fig. 16 illustrates the measured repose angles for each sample. It can be seen from the results

404   that the spherical aggregates have the smallest repose angle (15°), the ellipsoid aggregates have

405   an intermediate repose angle (28°), and the real crushed rock aggregates have the largest repose

406   angle (37°). This trend occurs because more elongated and more irregular-shaped aggregates

407   tend to have more considerable rolling resistance.

408   (2) The mean coordination number, Z, is a scalar parameter that provides macroscopic

409   information on the internal structural features (fabric) of granular materials. The evolution of

410   Z during baffle lifting and rock collapsing for all assemblies is illustrated in Fig. 17. In all cases,

411   Z exhibits a gradual drop versus the increasing simulation time during the aggregate collapsing

412   stage. When the aggregates form a stable heap, Z slightly increases and then reaches a stable

413   value. Among the three samples, sample S3 (with real crushed rocks) always exhibits larger

414   values of Z during the whole testing period, compared with S1 (with smallest Z) and S2 (with

415   intermediate Z). The results for Z reveal that more irregular-shaped aggregates tend to have

416   denser packing structures during the test. Besides, S1 (spherical aggregates) shows an earlier

417   drop at the initial stage, while the samples with more irregular aggregate shapes show more

418   delayed decreasing trends.

419   (3) The rotation motions are governed by the rolling resistance of the aggregates. In the

420   simulated repose angle tests, the rotational movements of the aggregates during collapsing

421   mostly occur around the x-axis. Thus, the mean accumulated rotational displacement around

422   the x-axis, ϑ_x, is computed. The results, as shown in Fig. 18, display the evolution of ϑ_x

423   versus simulation times for different samples. In general, for all numerical cases, the ϑ_x values

424   increase during the repose angle tests. For sample S1, the ϑ_x of spherical aggregates rises

425   sharply and gradually converges to a stable value. For samples S2 and S3, the ϑ_x of ellipsoid

426   and crushed rocks increase gradually and converge to a relatively small amount. It can be seen

427   in the figure that aggregate shapes play a significant role in the rotational movements. During

428   the whole process of the repose angle test, the spherical aggregates (AR=1.0) always exhibit a

429   significantly larger ϑ_x, at approximately 5 times the value for the ellipsoids (AR=0.65) and 7

430   times the value for the crushed rocks (AR=0.65).

4.3 Triaxial shear tests of real crushed rock aggregates

The macroscopic and microscopic properties of rock particle assemblies are of great importance to the engineering behaviors of the geo-body and the construction-body, e.g., slope, foundation, embankment, etc. Many researchers have reported that there are many factors, such as confining pressure, initial void ratio, and particle shape, that can significantly influence on the macro- and micromechanical properties of crushed rocks. In this section, three simulation groups of triaxial shear tests on realistic crushed rocks are performed to numerically examine the effect of confining pressure, preshear void ratio, and particle shapes. Group A consists of three samples with confining pressures of 50 kPa, 100 kPa, and 200 kPa, respectively. Group B consists of three samples with various initial void ratios prepared by preshear contact friction of 0.00, 0.15, and 0.30. Group C consists of three samples with various mean aspect ratios ($\overline{AR} = 0.95, 0.80, 0.65$). Fig. 19 shows the ranges of shapes and snapshots of crushed rock examples in Group C. The procedure to conduct a triaxial shear test in the SH-DEM is summarized as follows:

(1) For the random allocation of non-overlapped particles, the particle models of crushed rocks in the "STL" file format are first imported into the spherical harmonic transformation subroutine of the present SH-DEM program to obtain the harmonic coefficients for each particle. Then, as shown in Fig. 20 (*a*), nonoverlapping particles are allocated into a prescribed sample domain, which is a cubic container consisting of six rigid walls. Each sample consisted of approximately 1500 particles of monodispersed sizes ($d_{ave} = 20\ mm$).

451 (2) In the stage of isotropic compression, before activating external force to the assembly, the

452 properties of the material are assigned to all particles and walls to facilitate dynamic modeling

453 in the SH-DEM. The input parameters are consistent with those used in the former section for

454 real crushed rocks, except the wall friction (μ_{wall}=0 and $\mu_{particle}$=0.5) and the preshear contact

455 friction between particles ($\mu_{preshear}$=0 for Groups A and C, $\mu_{preshear}$=0, 0.15, 0.30 for Group

456 B). The gravitational force is set as zero during the simulation. Then, the consolidation

457 procedure is performed with the given confining stress to enable the assembly to reach an

458 isotropic stress state. The stress-control wall servo scheme is employed to move the six rigid

459 walls to maintain constant confining pressure, which shows an example of the preshear

460 numerical samples of crushed rocks in the SH-DEM. Fig. 20 (*b*) shows an example of the

461 preshear numerical sample of crushed rocks in the SH-DEM.

462 (3) During the triaxial shear stage, both the top and bottom walls move toward each other at a

463 constant strain rate, while the four lateral sidewalls move individually to maintain a constant

464 confining stress with the stress-control servo. The shear strain rate is set sufficiently low to

465 obtain quasi-static behavior during shearing. Fig. 20 (*c*) shows an example of a numerical rock

466 aggregate sample at shear strain of 50% in the SH-DEM.

467 In the present simulation, both macroscopic properties, e.g., deviatoric stress q, volumetric

468 strain ε_v, and microscopic quantities, e.g., mean coordination number, and percentage of

469 sliding contact are calculated at different axial strains ε_a. The results are detailed and discussed

470 as follows:

471 (1) The deviatoric stress q is computed to study the shear strength of the assemblies.

472 Fig. 21 shows the deviatoric stress q as a function of axial strain ε_a for all specimens with

473 different AR, preshear contact friction, and confining pressure. For specimens with different

474 AR, all curves behave in a similar fashion, showing peak stress, i.e., the stress softening. AR

475 tends to have a greater influence on postpeak behaviors. For peak state, the sample with AR=0.8

476 has the highest deviatoric stress, while in the residual state, the deviatoric stress increases with

477 the smaller value of AR. For specimens with different preshear contact friction, the smaller

478 value of PF leads to stress softening, while a larger value of PF leads to stress hardening. For

479 the peak state, the deviatoric stress increases with decreasing PF, while in the residual state, PF

480 shows a negligible influence on the deviatoric stress. For specimens with different confining

481 pressures, all curves show significant peak deviatoric shear stress.

482 (2) The volumetric changes of different specimens during shearing are investigated. Given that

483 the present cubic samples are bounded by rigid walls, the axial strain ε_1 and the volumetric

484 strain ε_v can be approximately calculated based on the displacement of the boundary walls.

485 As shown in Fig. 22, for groups A and C, the volumetric strain increases with increasing axial

486 strain, and the specimens deform at constant volume after reaching the critical state at an axial

487 strain ranging from 40% to 50%, which indicates that all specimens display shear-induced

488 dilatancy behavior with stress softening. For Group B, according to the difference between the

489 volumetric strain at the initial and residual states, the total volume change during shearing

490 appears to increase as PF decreases, indicating that an assembly with a smaller preshear contact

491 friction shows higher dilatancy during shearing.

492 (3) The coordination number is a scalar parameter that provides macroscopic information on

493 the internal structural features (fabric) of granular materials. The mean coordination numbers

494 of all samples, Z, are computed and compared. The evolution of Z against axial strain for all

495 assemblies is illustrated in Fig. 23. In all cases, Z exhibits an exponential drop versus the

496 increasing axial strain during the initial shearing process. When the axial strain is larger than

497 10%, Z reaches a low plateau with small fluctuations.

498 For Group A, the values of Z are always positively related to AR during the whole shear

499 process, i.e., Z increases from 7 to 8 at the initial state and shifts from 4.3 to 5.7 at the residual

500 state when AR varies from 0.65 to 0.95. For Group B, Z is only negatively related to PF during

501 the initial shear process. At the initial state, Z increases from 5.3 to 7.2 when PF decreases

502 from 0.3 to 0.0. When shear strain is larger than 10%, all samples with different PF show the

503 same values of Z and converge to a constant value of about 4.7. As for Group C, similar to

504 Group A, the values of Z are always positively related to the CP during the whole shear process.

505 The values of Z vary from 7.1 to 7.6 at the initial state and shift from 4.2 to 4.9 at residual

506 state when CP increases from 50 kPa to 200 kPa.

507 Besides, the sliding contacts are governed by Coulomb's friction law. We can denote the sliding

508 ratio (R_{sc}) using the ratio between shear force f_t and normal force f_n at each contact:

$$R_{sc} = |f_t|/(\mu_c f_n) \tag{24}$$

509 We assumed that sliding event occurs at contact when $R_{sc} > 0.99$. Then, the percentage of

510 sliding contact P_{sc} can be defined as:

$$P_{sc} = \sum_{i=1}^{N_c} G(R_{sc}) \Big/ N_c$$

(25)

$$G(R_{sc}) = \begin{cases} 0 & R_{sc} \leq 0.99 \\ 1 & R_{sc} > 0.99 \end{cases}$$

511   where N_c is the total number of contacts.

512   Fig. 24 displays the evolution of P_{sc} versus axial strain ε_a. In general, for all numerical cases,

513   P_{sc} increases sharply to a peak value, and then gradually decreases to a steady state.

514   Additionally, for Group A, P_{sc} increases from 59% to 70% at the peak state, and increases

515   from 40% to 47% at the steady state, when AR increases from 0.65 to 0.95. For Group B, the

516   samples only show negative relationships between peak P_{sc} and PF, i.e., P_{sc} increases from

517   55% to 65% when PF decreases from 0.3 to 0.0. The preshear contact friction shows the

518   negligible influence on P_{sc} at a steady state. For Group C, compared with AR and PF, CP

519   shows less influence on P_{sc}.

520   5 Conclusion

521   In this paper, a novel 3D SH-DEM approach has been developed for the simulation of 3D

522   realistic irregular-shaped particles. In the 3D SH-DEM, the spherical harmonic transformation

523   is first employed to represent particle shape in the local spherical coordination system. Then,

524   using the SH-based particle model, the intrinsic physical properties can be easily computed.

525   The novel numerical algorithms for identification of particle overlapping and contact

526   resolutions are developed based on the spherical harmonic function and the node-to-surface

527   scheme. The innovative features of the computational algorithms in the proposed 3D SH-DEM

528   are summarized as follows:

529   (*a*) The overlapping detection between SH-based irregular-shaped particles is implemented by

530   conventional global overlapping detection and unique local overlapping detection.

531   Conventional global overlapping detection is conducted by the combination of AABBs and the

532   spatial bins algorithm. The unique local overlapping detection is accomplished by (1)

533   discretizing the master particle into surface vertices, (2) substituting the discretized surface

534   vertices into the local spherical coordinate of slave particle, and (3) determining the penetration

535   condition of discretized surface vertices based on the spherical harmonic function of the slave

536   particle.

537   (*b*) The contact points are defined as the midpoints of the penetration vertices on the master

538   particle surface and the corresponding vertices on the slave particle surface with the same polar

539   angle at the local spherical coordinate system of the slave particle. The contact normal vector

540   at each contact is determined by the combination of the surface normal vectors of both the

541   master penetration vertices and corresponding vertices on the slave particle, which can be easily

542   and accurately computed based on the spherical harmonic functions.

543   (*c*) To determine the contact stiffness, the overlapping volume at each contact is computed based

544   on the local polyhedra, which are formed by the target penetration vertex and its one-ring

545   neighboring vertices.

546   Using the developed approach, three numerical examples were conducted to illustrate its

547   feasibility and capability. The simulation results are summarized as follows:

548   (*a*) Through simulations of the random deposition of superellipsoids with various shapes, the

549   evolutions of packing densities versus particle shapes are investigated and found to be

550   qualitatively consistent with the existing literature. The numerical results indicate that the

551   present SH-DEM model is reasonable for the simulation of non-spherical particles.

552   (*b*) Through simulating repose angle tests of realistic rock aggregates, it is indicated that the

553   contact friction coefficient between rocks should be taken as around 0.3 to simulate the realistic

554   repose angle of rocks in SH-DEM. Besides, the shape effects on macro- and micromechanical

555   properties of rock aggregate assemblies are primarily investigated through numerical repose

556   angle tests of spheres (AR=1.0), ellipsoids (AR=0.6), and realistic rock aggregates (AR=0.6)

557   using the SH-DEM. The shape effects on the angles of repose, mean coordination numbers, and

558   rotational motions are presented and compared.

559   (*c*) Through triaxial tests on rock aggregate assemblies, the effects of preshear contact friction,

560   particle aspect ratio, and confining pressure on the macroscopic and microscopic properties of

561   rock aggregates are presented. The simulation results of repose angle tests and triaxial tests

562   demonstrate that the developed SH-DEM approach is useful to investigate the shape effects on

563   the mechanical behaviors of realistic granular materials.

564   Indeed, compared with the simplified shape models such as disk-clump, the proposed method

565   can consider more realistic contact mechanics between irregular shape particles. The capability

566   and efficiency of the proposed SH-DEM program will pave a viable pathway for the researchers

567   to conduct more quantitative and credible studies on how the realistic particle shapes would

568   affect the macro- and micro-mechanical properties of granular materials. The method will be

569   further be developed to incorporate more advanced computational algorithms, e.g., the effective

570   energy-conserving contact modelling strategy [55], as future work.

571

575

576 **References**

577 [1] Su, D., & Yan, W. M. 2018. 3D characterization of general-shape sand particles using microfocus
578   X-ray computed tomography and spherical harmonic functions, and particle regeneration using
579   multivariate random vector. Powder Technology, 323, 8-23.

580 [2] Garboczi, E. J., & Bullard, J. W. 2013. Contact function, uniform-thickness shell volume, and
581   convexity measure for 3d star-shaped random particles. Powder Technology, 237, 191–201.

582 [3] Su, D., Wang, X., Yang, H., & Hong, C. Y. 2019. Roughness analysis of general-shape particles,
583   from 2D closed outlines to 3D closed surfaces. Powder Technology. 356, 423-438

584 [4] Cho, G. C., Dodds, J., & Santamarina, J. C. 2006. Particle shape effects on packing density, stiffness,
585   and strength: natural and crushed sands. Journal of geotechnical and geoenvironmental engineering,
586   132(5), 591-602.

587 [5] Nie, Z.H., Liang, Z.Y., & Wang, X. 2018. A three-dimensional particle roundness evaluation
588   method. Granular matter. 20:31.

589   [6] Zhigang, Zhu, Huisu, Chen, Wenxiang, & Xu, et al. (2014). Parking simulation of three-
590   dimensional multi-sized star-shaped particles. Modelling and Simulation in Materials Science and
591   Engineering, 22(3), 35008-35008.

592   [7] Ting, J. M., Meachum, L., & Rowell, J. D. 1995. Effect of particle shape on the strength and
593   deformation mechanisms of ellipse-shaped granular assemblages. Engineering Computations,
594   12(2), 99-108.

595   [8] Lin, X., & Ng, T. T. 1995. Contact detection algorithms for three-dimensional ellipsoids in discrete
596   element modelling. International Journal for Numerical and Analytical Methods in Geomechanics,
597   19(9), 653-659.

598   [9] Lin, X., & Ng, T. T. 1997. A three-dimensional discrete element model using arrays of ellipsoids.
599   Geotechnique, 47(2), 319-329.

600   [10] Azéma, E., & Radjai, F. 2010. Stress-strain behavior and geometrical properties of packings of
601   elongated particles. Physical Review E, 81(5), 051304.

602   [11] Azéma, E., & Radjai, F. 2012. Force chains and contact network topology in sheared packings of
603   elongated particles. Physical review E, 85(3), 031303.

604   [12] Lu, P., Li, S., Zhao, J., & Meng, L. 2010. A computational investigation on random packings of
605   sphere-spherocylinder mixtures. Science China Physics, Mechanics and Astronomy, 53(12), 2284-
606   2292.

607   [13] Zhao, S., Zhang, N., Zhou, X., & Zhang, L. 2017. Particle shape effects on fabric of granular
608   random packing. Powder technology, 310, 175-186.

609   [14] Han, K., Feng, Y. T., & Owen, D. R. J. 2006. Polygon-based contact resolution for superquadrics.
610   International journal for numerical methods in engineering, 66(3), 485-501.

611   [15] Zhou, W., Huang, Y., Ng, T. T., & Ma, G. 2018. A geometric potential-based contact detection
612   algorithm for egg-shaped particles in discrete element modeling. Powder Technology, 327, 152-
613   162.

614   [16] Munjiza, A., Peters, J. F., Hopkins, M. A., Kala, R., & Wahl, R. E. 2009. A poly-ellipsoid particle
615   for non-spherical discrete element method. Engineering Computations.

616   [17] Zhao, S., & Zhao, J. 2019. A poly-superellipsoid-based approach on particle morphology for DEM
617   modeling of granular media. International Journal for Numerical and Analytical Methods in
618   Geomechanics, 43(13), 2147-2169.

619   [18] Feng, Y. T., & Owen, D. R. J. 2004. A 2D polygon/polygon contact model: algorithmic aspects.
620   Engineering Computations.

621   [19] Feng, Y.T., Tan, Y.Q., 2019. On Minkowski difference-based contact detection in
622   discrete/discontinuous modelling of convex polygons/polyhedra. Engineering Computations, 37(1),
623   54-72.

624   [20] Zhao, S., Zhao, J. 2020. SudoDEM : unleashing the predictive power of the discrete element method
625   on simulation for non-spherical granular particles. Computer Physics Communications.

626   [21] Ferellec, J. F., & McDowell, G. R. 2008. A simple method to create complex particle shapes for
627   DEM. Geomechanics and Geoengineering: An International Journal, 3(3), 211-216.

628   [22] Zheng, J., & Hryciw, R. D. 2017. An image based clump library for DEM simulations. Granular
629   Matter, 19(2), 26.

630   [23] Yan, W. M. 2010. Particle elongation and deposition effect to macroscopic and microscopic
631   responses of numerical direct shear tests. Geotechnical Testing Journal, 34(3), 238-249.

632   [24] Nie, Z., Zhu, Y., Wang, X., & Gong, J. 2019. Investigating the effects of Fourier-based particle
633   shape on the shear behaviors of rockfill material via DEM. Granular Matter, 21(2), 22.

634   [25] Kodam, M., Bharadwaj, R., Curtis, J., Hancock, B., & Wassgren, C. 2009. Force model
635   considerations for glued-sphere discrete element method simulations. Chemical Engineering
636   Science, 64(15), 3466-3475.

637   [26] Höhner, D., Wirtz, S., Kruggel-Emden, H., & Scherer, V. 2011. Comparison of the multi-sphere
638   and polyhedral approach to simulate non-spherical particles within the discrete element method:
639   Influence on temporal force evolution for multiple contacts. Powder Technology, 208(3), 643-656.

[27] Li, Z.F. 2017. Validations and applications of discrete element method. The Hong Kong University of Science and Technology: Hong Kong.

[28] Andrade, J. E., Lim, K. W., Avila, C. F., & Vlahinić, I. 2012. Granular element method for computational particle mechanics. Computer Methods in Applied Mechanics and Engineering, 241, 262-274.

[29] Liu, S., Chen, F., Ge, W., & Ricoux, P. 2020. NURBS-based DEM for non-spherical particles. Particuology, 49, 65-76.

[30] Kawamoto, R., Andò, E., Viggiani, G., & Andrade, J. E. 2018. All you need is shape: Predicting shear banding in sand with LS-DEM. Journal of the Mechanics and Physics of Solids, 111, 375-392.

[31] Lai, Z., Chen, Q., & Huang, L. 2020. Fourier series-based discrete element method for computational mechanics of irregular-shaped particles. Computer Methods in Applied Mechanics and Engineering, 362, 112873.

[32] Feng, Y.T., Han, K., Owen, D.R.J. Energy-conserving contact interaction models for arbitrarily shaped discrete elements. Computer Methods in Applied Mechanics & Engineering, 2012. 205-208: 169-177.

[33] Feng, Y. T. An energy-conserving contact theory for discrete element modelling of arbitrarily shaped particles: basic framework and general contact model. Computer Methods in Applied Mechanics and Engineering, 2021, 373, 113454.

[34] Feng, Y.T. An energy-conserving contact theory for discrete element modelling of arbitrarily shaped particles: Contact volume based model and computational issues. Computer Methods in Applied Mechanics and Engineering, 2021. 373, 113493.

[35] Farsi, A., Xiang, J., Latham, J. P., Carlsson, M., & Marigo, M. 2020. Packing simulations of complex-shaped rigid particles using FDEM: an application to catalyst pellets. Powder Technology, 380(8).

665 [36] Joulin, C., Xiang, J., Latham, J. P., Pain, C., Salinas, P. 2020. Capturing heat transfer for complex-

666 shaped multibody contact problems, a new FDEM approach. Computational Particle Mechanics,

667 7(5), 919-934.

668 [37] Latham, J.P., Xiang, J., Farsi, A., Joulin, C., & Karantzoulis, N. 2019. A class of particulate

669 problems suited to FDEM requiring accurate simulation of shape effects in packed granular

670 structures. Computational Particle Mechanics, 1-12.

671 [38] Munjiza, A., Rougier, E., Zhou, L., & Knight, E. E. 2020. FSIS: a novel fluid–solid interaction

672 solver for fracturing and fragmenting solids. Computational Particle Mechanics, 7(4).

673 [39] Thornton, C. 1992. Applications of DEM to process engineering problems. Engineering

674 Computations, 9(2), 289-297.

675 [40] Xiang, J., Munjiza, A., Latham, J.P., Guises, R. 2009. On the validation of DEM and FEM/DEM

676 models in 2D and 3D. Engineering Computations, 26(6), 673-687.

677 [41] Latham, J.P., Munjiza, A. 2004. The modelling of particle systems with real shapes. Philosophical

678 Transactions: Mathematical, Physical and Engineering Sciences, 362(1822), 1953-1972.

679 [42] Laursen, T., 2002. Computational Contact and Impact Mechanics: Fundamentals of Modeling

680 Interfacial Phenomena in Nonlinear Finite Element Analysis. Springer, Berlin.

681 [43] Puso, M. A., & Laursen, T. A. 2002. A 3D contact smoothing method using Gregory patches.

682 International Journal for Numerical Methods in Engineering, 54(8), 1161-1194.

683 [44] Lim, K.-W., Krabbenhoft, K., Andrade, J., 2014. On the contact treatment of non-convex particles

684 in the granular element method. Computational Particle Mechanics. 1 (3), 257–275.

685 [45] Zhao, S., Zhou, X., & Liu, W. 2015. Discrete element simulations of direct shear tests with particle

686 angularity effect. Granular Matter, 17(6), 793-806.

687 [46] Donev, A., Cisse, I., Sachs, D., Variano, E. A., Stillinger, F. H., Connelly, R., & Chaikin, P. M.

688 2004. Improving the density of jammed disordered packings using ellipsoids. Science, 303(5660),

689 990-993.

690   [47] Zhou, Z. Y., Zou, R. P., Pinson, D., & Yu, A. B. 2011. Dynamic simulation of the packing of
691   ellipsoidal particles. Industrial & engineering chemistry research, 50(16), 9787-9798.

692   [48] Jiao, Y., Stillinger, F. H., & Torquato, S. 2009. Optimal packings of superballs. Physical Review
693   E, 79(4), 041309.

694   [49] Delaney, G. W., & Cleary, P. W. 2010. The packing properties of superellipsoids. EPL
695   (Europhysics Letters), 89(3), 34002.

696   [50] Williams, J.R., Pentland, A.P. 1992. Superquadrics and modal dynamics for discrete elements in
697   interactive design. Engineering Computations, 9(2), 115-127.

698   [51] Owen, D. R. J. 2004. A Robust Contact Model for Rigid Super-Quadrics. In Abstracts of the Papers
699   Presented at the Regular Sessions of the Sixth World Congress on Computational Mechanics in
700   Conjunction with the Second Asian-Pacific Congress on Computational MechanicsII.

701   [52] Munjiza, A., And, D., & Crook, A. 1998. An $M(M^{-1}K)^m$ proportional damping in explicit
702   integration of dynamic structural systems. International Journal for Numerical Methods in
703   Engineering, 41, 1277–1296.

704   [53] Munjiza, A. 2004. The combined finite-discrete element method. John Wiley & Sons.

705   [54] Munjiza, A. Latham, J.P., & John, N. 2003. 3D dynamics of discrete element systems comprising
706   irregular discrete elements—integration solution for finite rotations in 3D. International Journal for
707   Numerical Methods in Engineering, 56(1).

708   [55] Feng, Y.T. An effective energy-conserving contact modelling strategy for spherical harmonic
709   particles represented by surface triangular meshes with automatic simplification. Comput. Methods
710   Appl. Mech. Engrg. 2021, 379: 113750.

711

712 **Tables**

713

714 <center>**Table 1** DEM simulation parameters</center>

Parameter	Value
Particle density, ρ (kg/m^3)	2700
Damping coefficient, α	0.3
Volumetric normal contact stiffness, k_n (N/m^3)	1×10^{11}
Shear contact stiffness, k_t (N/m)	1×10^7
Contact friction	0.48

715

716

717

Appendix A   Motion of particles in SH-DEM

In the proposed SH-DEM, for each particle, the motion can be divided into two parts: translation in the global coordinate system and rotation in the local coordinate system. To facilitate numerical processing, the global coordinate system is usually the world coordinate system of the particle system, while the local coordinate system is fixed on the individual particle and moves synchronously with the particle.

The translational motion of a particle in the global coordinate system is governed by Newton equations:

$$m\frac{d\boldsymbol{v}_i}{dt} = \boldsymbol{F}_i \tag{A1}$$

where m is the particle mass; $\boldsymbol{v}_i$ is the translational velocity along the i axis of the global coordinate system; $i \in \{1,2,3\}$ represents the axis of the global coordinate system, and $\boldsymbol{F}_i$ is the total resultant force acting on the particle centroid (mass center), which can be calculated as:

$$\boldsymbol{F}_i = \sum_{k=1}^{N_c} \boldsymbol{F}_k^c + \boldsymbol{F}^b + \boldsymbol{F}^d \tag{A2}$$

where N_c is the contact number of the particle; $\boldsymbol{F}^b$ is the body force, e.g., gravitational force; $\boldsymbol{F}^d$ is the damping force; and $\boldsymbol{F}_k^c$ is the contact force acting at the k_{th} contact.

Compared with the contact force between the spherical particles, a remarkable feature of the contact force between irregular-shaped particles is that the normal component of the contact force (normal contact force) usually does not pass through the particle's center of mass, so the torque around the center of mass can be generated. The torque can promote or inhibit the rotation of the irregular-shaped particle. In a local coordinate system, Euler's equations are applied to particle rotations:

$$I_i \frac{d\omega_i}{dt} - (I_j - I_k)\omega_j \omega_k = M_i \tag{A3}$$

738   where $i, j, k \in 1,2,3$ is the principal axis; I_i is the principal moment of inertia; ω_i is the

739   angular velocity, and M_i is the i_{th} component of the total resultant torque M, which can be

740   calculated as:

$$M = \sum_{k=1}^{N_c} F_k^c \times r_k + M^d \tag{A4}$$

741   where r_k is the radical vector of the k_{th} contact; and M^d is the damping moment.

742   To stabilize the system after a reasonable number of iterations, following general DEM codes,

743   artificial numerical damping is used to dissipate the kinetic energy. In this study, two types of

744   damping are facilitated: local damping and viscous damping. Local damping provides damping

745   to reduce the particle speed through adjustment of the resultant external force. Note that the

746   resultant force discussed here includes the resultant force moment, and the velocity includes

747   the angular velocity of rotation. Generally, a fixed coefficient, i.e., the damping coefficient, is

748   used to adjust the resultant external forces and a corresponding damping force F_i^d is added to

749   the right-hand side of the Newton equation and Euler's equations, given as:

$$F_i^d = -\alpha F_i \text{Sign}\left(F_i \left(v_i^{(t-\Delta t/2)} + \frac{dv_i^t}{dt} \frac{\Delta t}{2} \right) \right)$$

$$\tag{A5}$$

$$M_i^d = -\alpha M_i \text{Sign}\left(M_i \left(\omega_i^{(t-\Delta t/2)} + \frac{d\omega_i^t}{dt} \frac{\Delta t}{2} \right) \right)$$

750   where α is the damping coefficient; Δt is the time step; $v_i^{(t-\Delta t/2)}$ and $\omega_i^{(t-\Delta t/2)}$ are the

751   previous mid-step translational velocity and angular velocity, respectively; $\frac{dv_i^t}{dt}$ and $\frac{d\omega_i^t}{dt}$ are

752   the current on-step translational acceleration and angular acceleration, respectively; and

753    $\text{Sign}(x)$ is the signum function:

$$\text{Sign}(x) = \begin{cases} -1 & \text{if } x < 0, \\ 0 & \text{if } x = 0, \\ 1 & \text{if } x > 0. \end{cases} \tag{A6}$$

754   Viscous damping is a kind of damping applied at the contact of particles, which can reduce the

755   relative velocity of two contact particles by adjusting the contact force. The normal and

756   tangential viscous damping forces F_n^d and F_t^d are calculated by:

$$F_n^d = 2\sqrt{\overline{m}k_n}\beta_n V_n$$

$$\tag{A7}$$

$$F_t^d = 2\sqrt{\overline{m}k_t}\beta_t V_t$$

757   where $\overline{m} = m^M m^S / (m^M + m^S)$ is the equivalent mass of the two contacted particles; β_n

758   and β_t are the normal and tangential viscous damping coefficients, respectively; and V_n and

759   V_t are the normal and tangential components of the relative velocity of the two particles at the

760   contact. It should be noted that the viscous damping force should not exceed the corresponding

761   contact force. The Eq. (A7) is based on the previous work [45]. Similar approach can be referred

762   to [52][53].

763

Appendix B   Scheme of computation in SH-DEM

764

765   The computational iteration of the proposed SH-DEM includes two components: the particle

766   system and the contact system. In the particle system, the change in the particle position is

767   accompanied by the appearance or disappearance of interparticle contact. The computation

768   scheme can be concluded as: (1) Given the position of particles in the system, determine the

769   corresponding geometric information of the contact between particles through contact detection

770   between particles; (2) According to the given contact model, calculate the contact force at each

771   contact and the resulted moment acted on each particle; (3) Based on the given movement law

772   (Newton's second law), calculate the motion of the particles and drive the particles to the new

773   positions; (4) continue the next computation cycle from (1) to (3).

774   The so-called central difference method is done to solve the particle motion (Newton's and

775   Euler's equations. A brief description of the solution process of Newton's equation based on the

776   standard leapfrog algorithm is adopted.

777   (1) Given a specific position vector $\boldsymbol{x}^t$ at time t and the position vector $\boldsymbol{x}^{t-\Delta t}$ at time $t-$

778   Δt, calculate the translational velocity $\boldsymbol{v}^{t-\frac{\Delta t}{2}}$ at time $t-\frac{\Delta t}{2}$:

$$\boldsymbol{v}^{t-\frac{\Delta t}{2}} = \frac{\boldsymbol{x}^t - \boldsymbol{x}^{t-\Delta t}}{\Delta t} \tag{B1}$$

779   (2) Calculate the translational acceleration $\boldsymbol{a}^t$ at time t:

$$\boldsymbol{a}^t = \frac{\boldsymbol{F}}{m} \tag{B2}$$

780   (3) Calculate the translational velocity $\boldsymbol{v}^{t+\frac{\Delta t}{2}}$ at time $t+\frac{\Delta t}{2}$:

$$\boldsymbol{v}^{t+\frac{\Delta t}{2}} = \boldsymbol{v}^{t-\frac{\Delta t}{2}} + \boldsymbol{a}^t \Delta t \tag{B3}$$

781   (4) Calculate the position vector $\boldsymbol{x}^{t+\Delta t}$ at time $t+\Delta t$:

$$\boldsymbol{x}^{t+\Delta t} = \boldsymbol{x}^t + \boldsymbol{v}^{t+\frac{\Delta t}{2}} \Delta t \tag{B4}$$

782   For Euler's equations, based on the previous development [54], the extending leapfrog

783   algorithm is employed as follows:

784   (1) Given a specific angular momentum $L^{t-\frac{\Delta t}{2}}$ at time $t-\frac{\Delta t}{2}$ and external resultant moment

785   M^t at time t, the angular momentum at time t and $t+\frac{\Delta t}{2}$ can be calculated as:

$$L^t = L^{t-\frac{\Delta t}{2}} + M^t \frac{\Delta t}{2} \tag{B5}$$

$$L^{t+\frac{\Delta t}{2}} = L^{t-\frac{\Delta t}{2}} + M^t \Delta t \tag{B6}$$

786   (2) The corresponding local angular velocity $\widehat{\omega}^t$ at the local coordinate system can be

787   calculated by:

$$\widehat{\omega}^t = \boldsymbol{I}^{-1} T L^t \tag{B7}$$

$$\widehat{\omega}^{t+\frac{\Delta t}{2}} = \boldsymbol{I}^{-1}\boldsymbol{T}\boldsymbol{L}^{t+\frac{\Delta t}{2}} \tag{B8}$$

788   where T is the rotation matrix transformed from global coordinates to local coordinates at time

789   t, which can be obtained by the quaternion matrix q^t.

790   (3) The change rate of q^t with respect to time t, denoted as $\dot{q}^t$, can be calculated as:

$$\dot{q}^t = \begin{bmatrix} \dot{q}_\omega^t \\ \dot{q}_x^t \\ \dot{q}_y^t \\ \dot{q}_z^t \end{bmatrix} = \frac{1}{2}\begin{bmatrix} q_\omega^t & -q_x^t & -q_y^t & -q_z^t \\ q_x^t & q_\omega^t & -q_z^t & q_y^t \\ q_y^t & q_z^t & q_\omega^t & -q_x^t \\ q_z^t & -q_y^t & q_z^t & q_\omega^t \end{bmatrix}\begin{bmatrix} 0 \\ \widehat{\omega}_x^t \\ \widehat{\omega}_y^t \\ \widehat{\omega}_z^t \end{bmatrix} \tag{B9}$$

791   and the quaternion matrix $q^{t+\frac{\Delta t}{2}}$ can be calculated as:

$$q^{t+\frac{\Delta t}{2}} = q^t + \dot{q}^t\frac{\Delta t}{2} \tag{B10}$$

792   (4) The global angular velocity $\omega^{t+\frac{\Delta t}{2}}$ at time $t + \frac{\Delta t}{2}$ can be calculated by:

$$\omega^{t+\frac{\Delta t}{2}} = T^{-1}\widehat{\omega}^{t+\frac{\Delta t}{2}} \tag{B11}$$

793   The solution involves explicit finite difference with incremental time steps, which is dependent

794   on the incremental time step Δt. On the one hand, in the particle system, the movement of a

795   single particle at each time step needs to be small enough so that the movement of a single

796   particle only affects the surrounding particles. On the other hand, when using the central

797   difference method, the time step Δt needs to be small enough to keep the error in the particle

798   motion solution as small as possible. Therefore, scholars have put forward the concept of the

799   critical time step that the maximum time step should satisfy the numerical stability. However,

800   due to the complexity of the particle system, there is no unified theoretical derivation for the

801   determination of the critical time step. The smaller the time step is, the more accurate the

802   particle motion calculation is, and the more stable the numerical value is. The very accurate

803   calculation of the movement of each particle will not change (or improve) the simulation results

804   substantially, but will significantly increase the calculation time, which is obviously of no

805   practical significance. Hence, to make simulation numerically stable, the present timestep in

806   this study will be tentatively selected based on empirical trials.

807

Figure captions

Fig. 1 The digitalized models of realistic rock particle: (a) triangular mesh model obtained from 3D laser scanning, (b) transform discrete surface vertices from Cartesian Coordinate to Spherical Coordinate, (c) continuously representation of the discrete particle surface using the spherical harmonic function
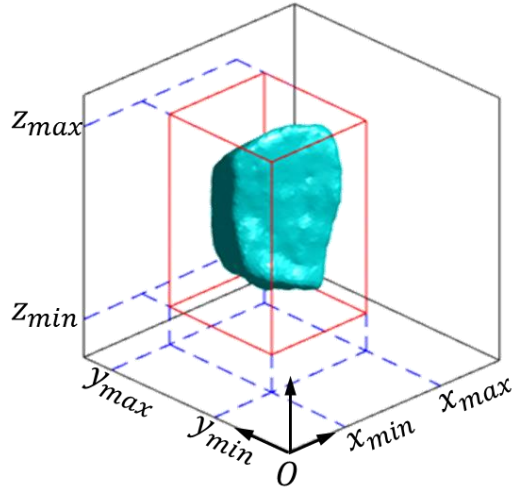
Fig. 2 AABB of an example particle in the global Cartesian coordinate system

Fig. 3 determine the potential overlapping range of spherical angles: (a) Circumscribed spheres of MG and SG, (b) Potential overlapping range
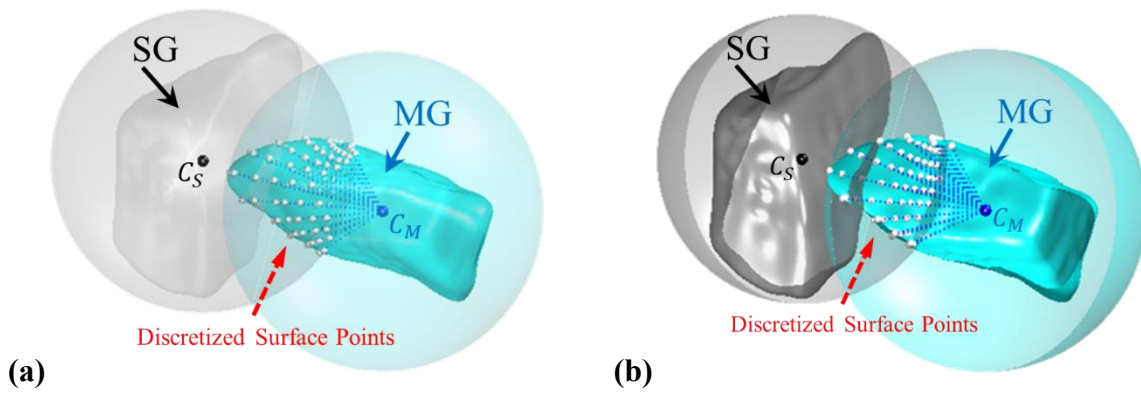
Fig. 4 Example of surface discretization with vertices in white seeded on the within the identified potential overlapping region: (a) full-space view, (b) half-space view
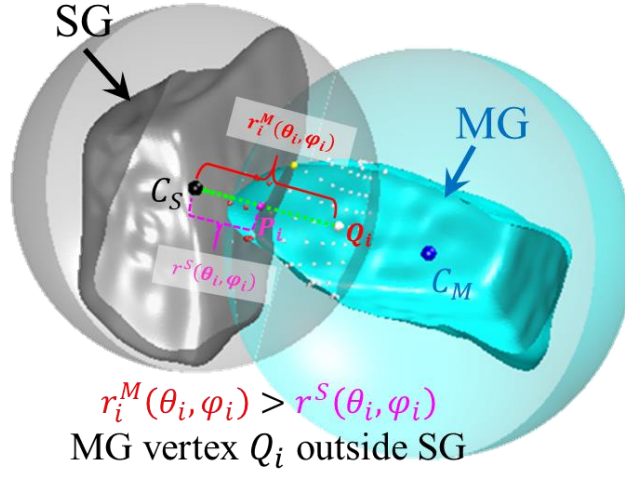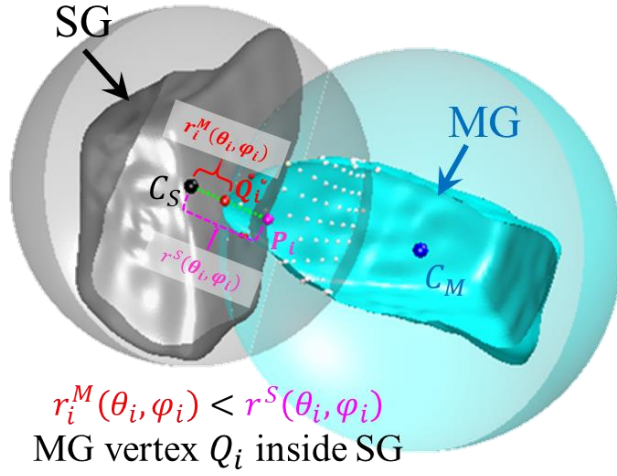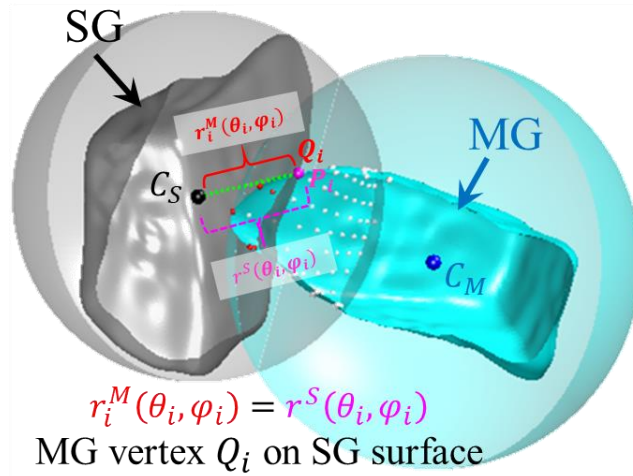
Fig. 5 Location of $Q_i'[r_i^{M'}(\theta'_i, \varphi'_i)]$ of MG with respect to SG: (a) when MG vertex Q_i outside SG, (b) when MG vertex Q_i inside SG, (a) when MG vertex Q_i on SG surface
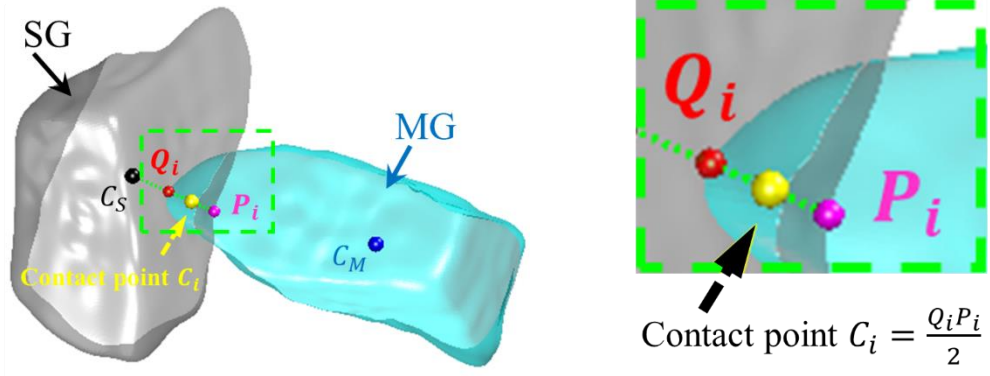
Fig. 6 Definition of contact point C_i for a pair of penetration points Q_i and P_i
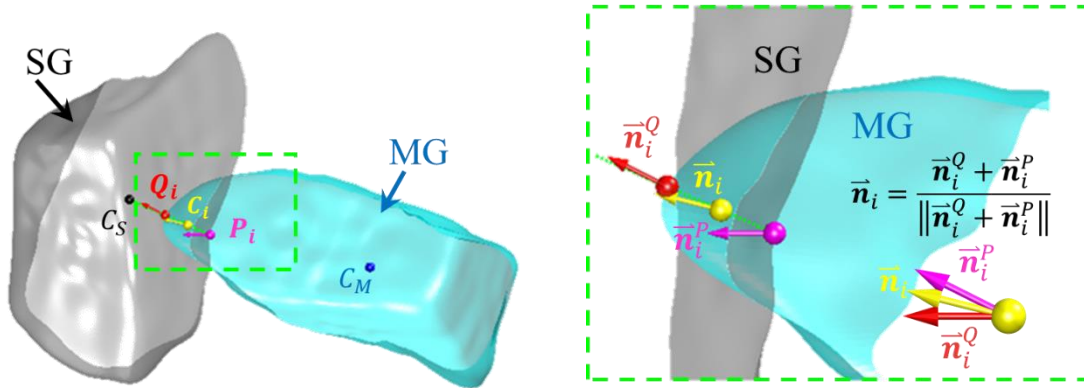
Fig. 7 Definition of contact normal vector $\vec{n}_i$ at contact point C_i
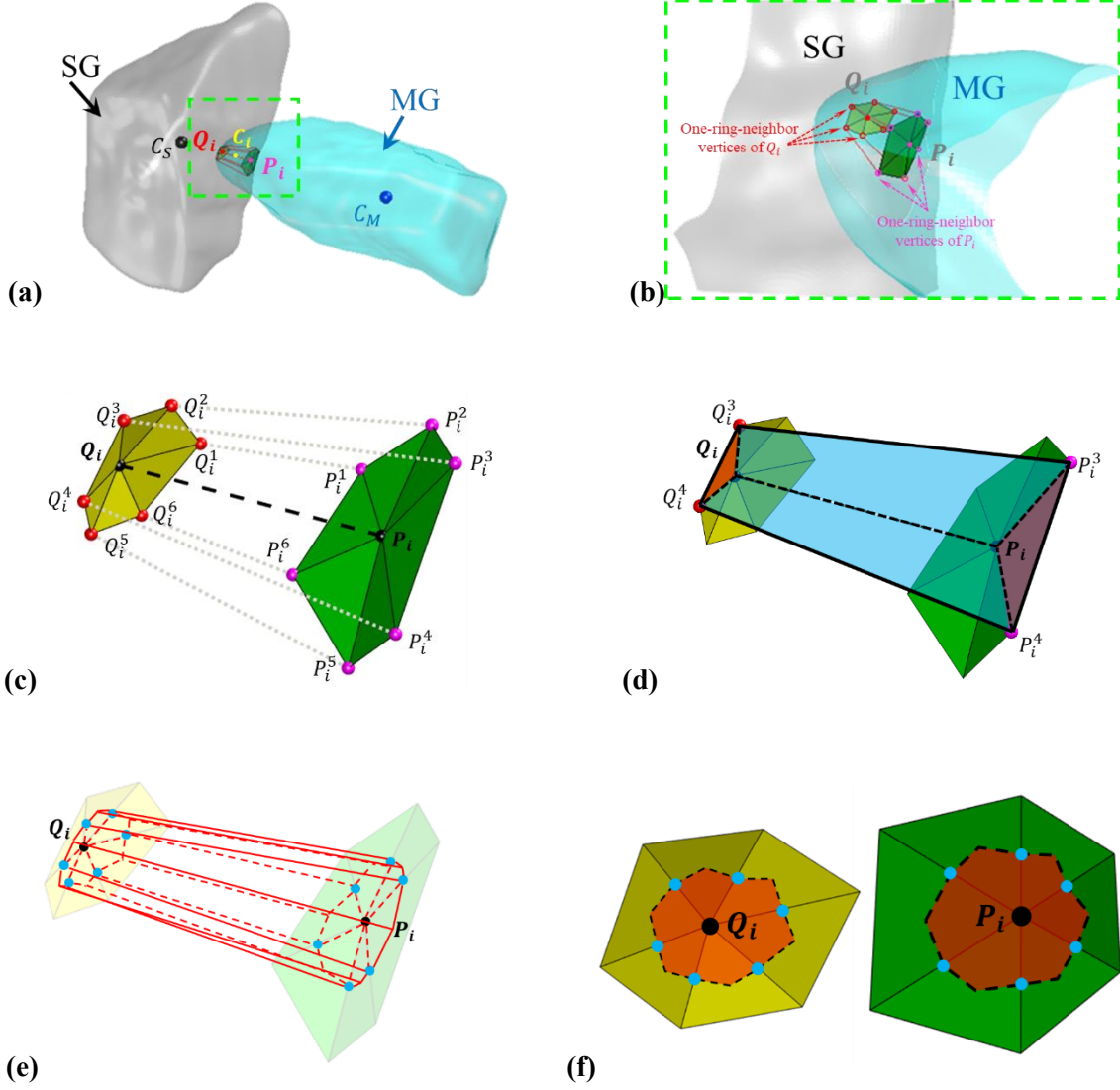
Fig. 8 Definition of local overlapping volume V_i at contact point C_i: (a) whole particle view, (b) local region view, (c) one-ring-neighbor vertices, (d) Example of $V_{P_i P_i^k P_i^{k+1} Q_i Q_i^k Q_i^{k+1}}$, (e) the local overlapping volume V_i, (f) the top and base facets of V_i
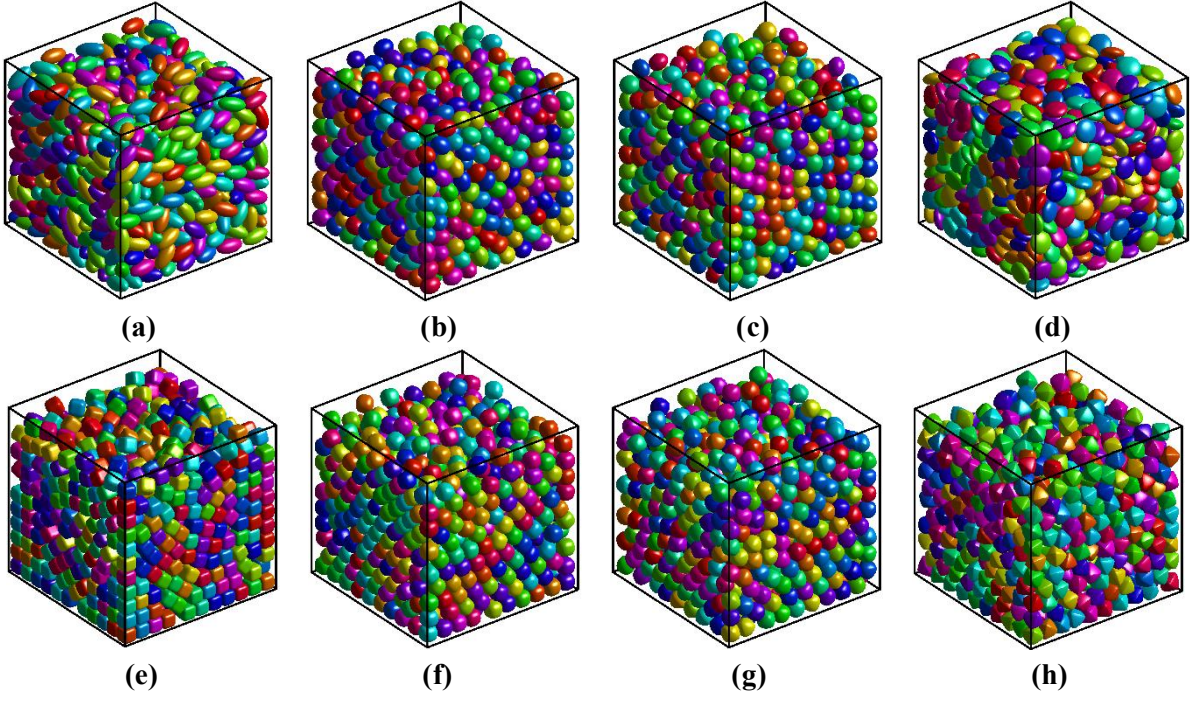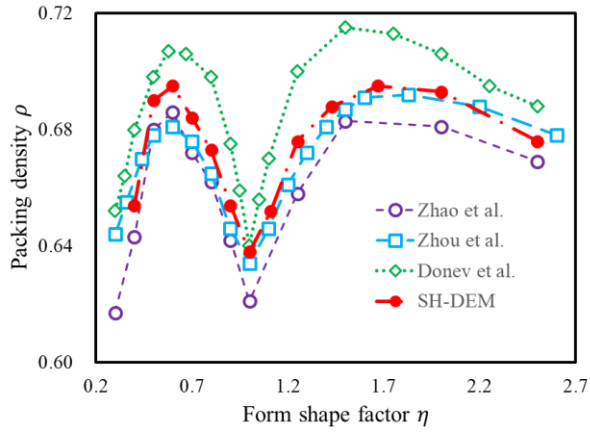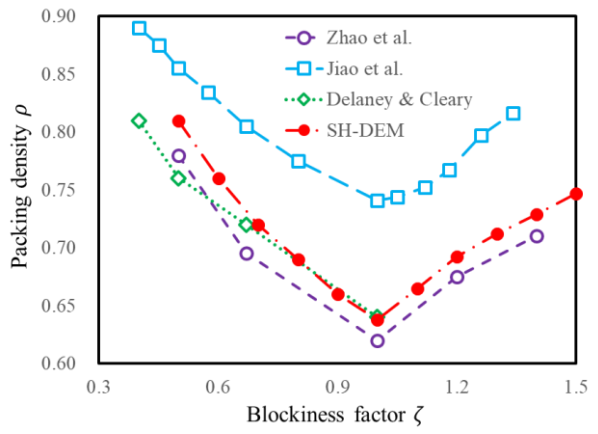
Fig. 9 Packing of some example superellipsoid particles (*a*) η=2.0; (*b*) η=1.25; (*c*) η=0.8; (*d*) η=0.5; (*e*) ζ=0.5; (*f*) ζ=0.8; (*g*) ζ=1.2; (*h*) ζ=1.5
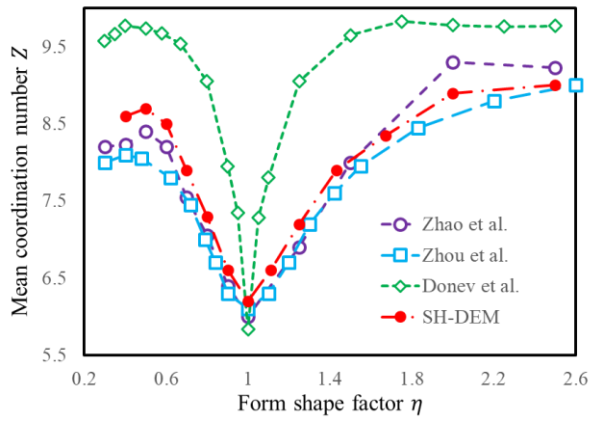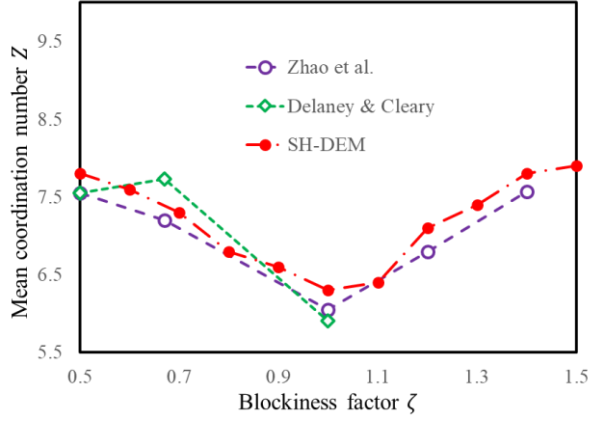
Fig. 10 Packing density for superellipsoid (a) with different η and (b) with different ζ

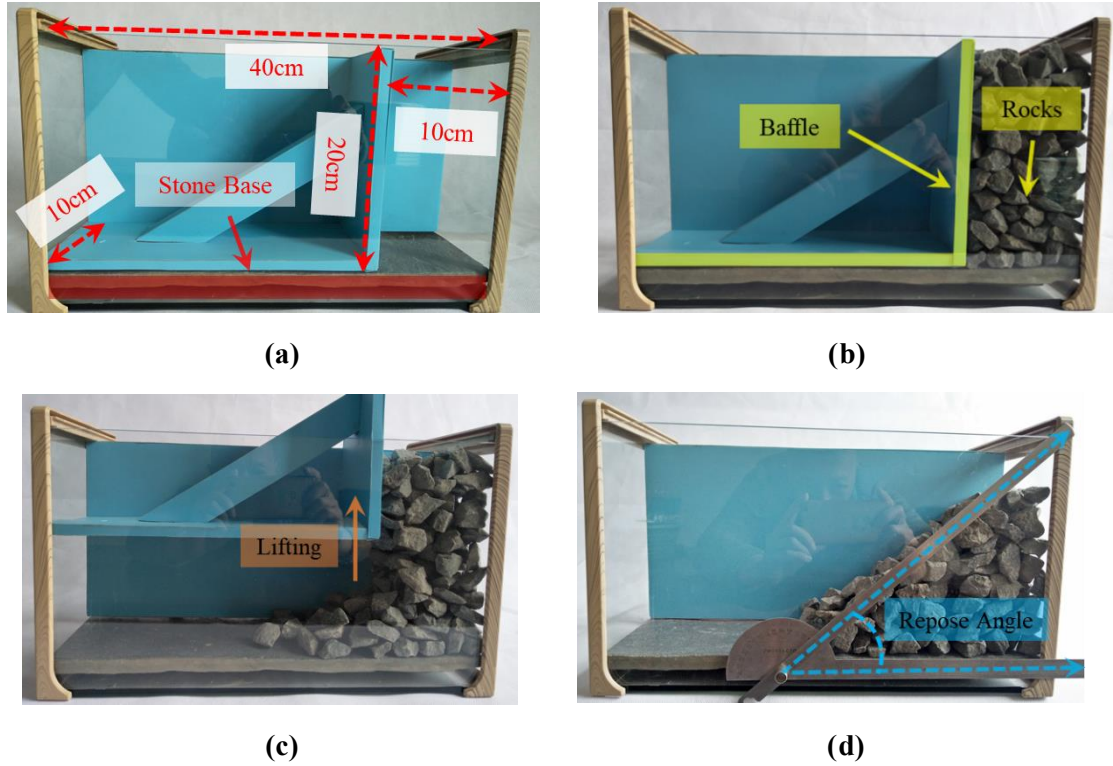Fig. 11 Mean coordination number Z for superellipsoid (a) with different η and (b) with different ζ

Fig. 12 Laboratory test of the angle of repose (a) container; (b) test step, (c) lift side-wall (d) measurement of the repose angle

Fig. 13 Illustration of (a) the real crushed rock for testing and (b) the 3D virtual model obtained by the 3D laser scanner
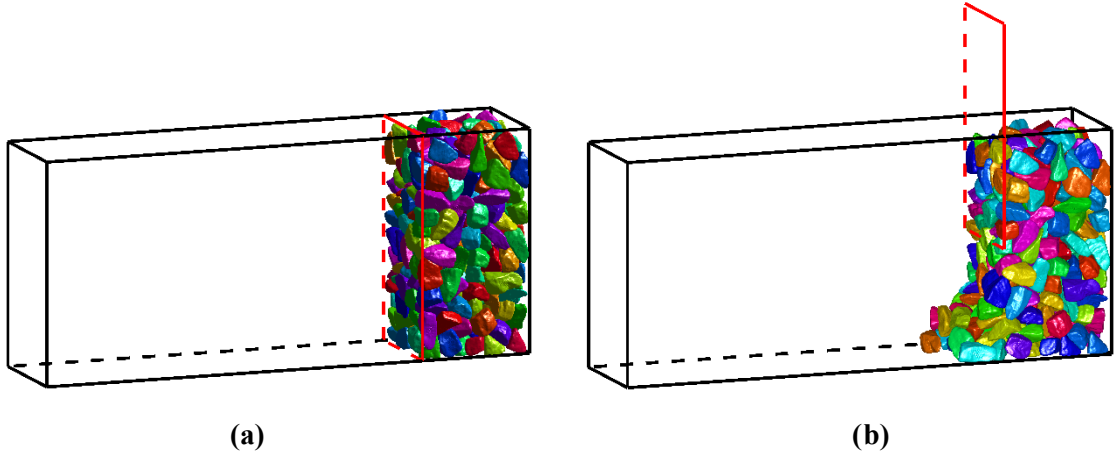
Fig. 14 Numerical test of repose angle in SH-DEM: (a) Initial sample; (b) During testing
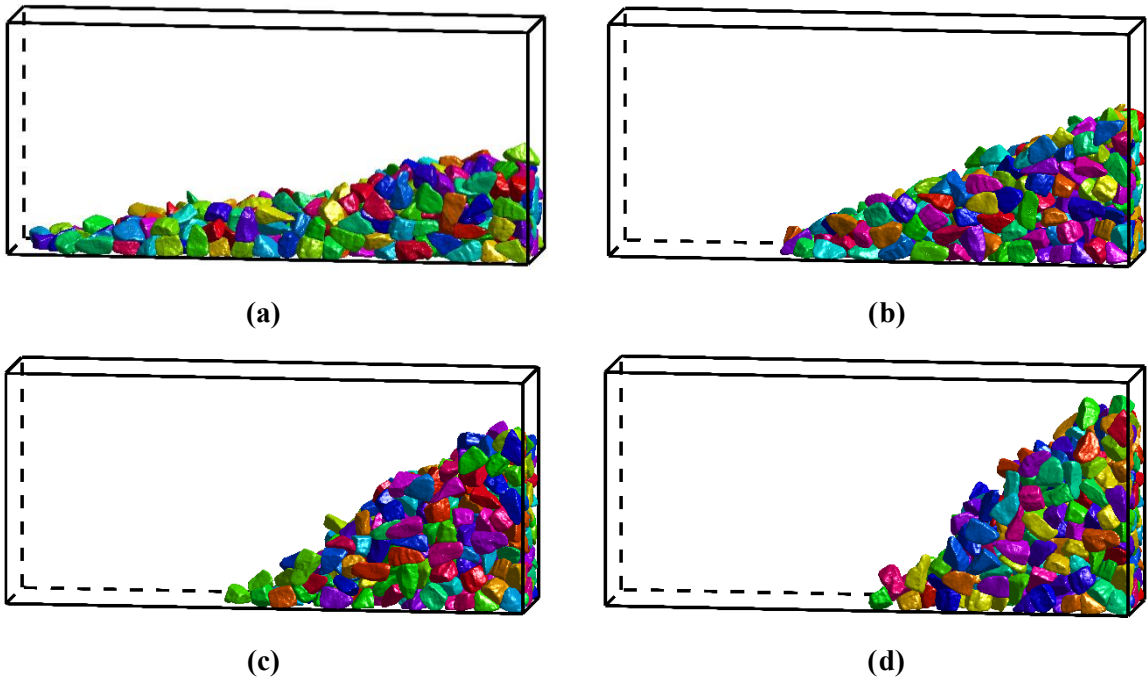
Fig. 15 Repose angles of samples with different contact friction coefficients: (a) contact friction = 0.1; (b) contact friction = 0.2; (c) contact friction = 0.3; (d) contact friction = 0.5
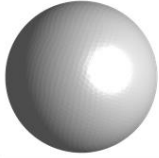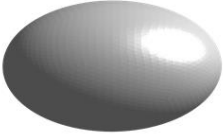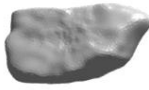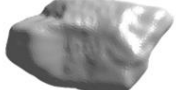
Fig. 16 Ranges of shapes and the snapshots of example crushed rocks

Fig. 17 Repose angles of samples with different particle shapes: (a) spherical particle with AR=1.0; (b) ellipsoid particle with AR=0.65; (c) crushed rocks with AR=0.65
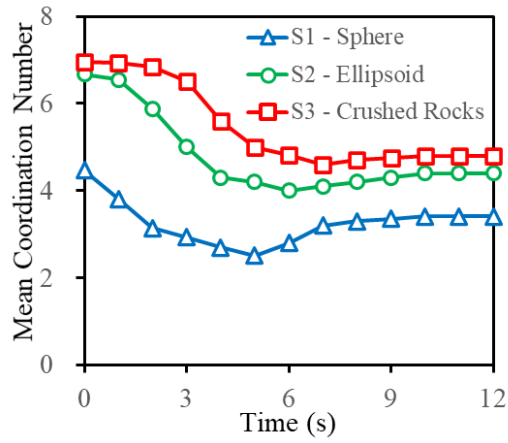
Fig. 18 Evolution of mean coordination number during repose angle tests for different samples

Fig. 19 Evolution of mean rotational displacement during repose angle tests for different samples

Fig. 20 Ranges of shapes and the snapshots of example crushed rocks in Group C

Fig. 21 (a) non-overlapped rock aggregates; (b) consolidated rock aggregate sample; (c) Sheared rock aggregate sample

Fig. 22 Comparison of deviatoric stress between (a) samples of different AR; (b) samples of different preshear contact friction; (c) samples of different confining pressure

Fig. 23 Comparison of volumetric strain between (a) samples of different AR; (b) samples of different preshear contact friction; (c) samples of different confining pressure

848   Fig. 24   Comparison of volumetric strain between (a) samples of different AR; (b) samples of different

849   preshear contact friction; (c) samples of different confining pressure

850   Fig. 25   Comparison of percentage of sliding contact between (a) samples of different AR; (b) samples

851   of different preshear contact friction; (c) samples of different confining pressure

852

853

854 **(a)**

855

856 **(b)**

857 **(c)**

858

859 Fig. 1 The digitalized models of realistic rock particle: (a) triangular mesh model obtained from 3D

860 laser scanning, (b) transform discrete surface vertices from Cartesian Coordinate to Spherical

861 Coordinate, (c) continuously representation of the discrete particle surface using the spherical

862 harmonic function

863

864

865   Fig. 2   AABB of an example particle in the global Cartesian coordinate system

866

867

868

869   **(a)**   **(b)**

870

871   Fig. 3   determine the potential overlapping range of spherical angles: (a) Circumscribed spheres of

872   MG and SG, (b) Potential overlapping range

873

874

875   **(a)**   **(b)**

876

877   Fig. 4   Example of surface discretization with vertices in white seeded on the within the identified

878   potential overlapping region: (a) full-space view, (b) half-space view

879

$$r_i^M(\theta_i, \varphi_i) > r^S(\theta_i, \varphi_i)$$
MG vertex Q_i outside SG

880
881

(a)

$$r_i^M(\theta_i, \varphi_i) < r^S(\theta_i, \varphi_i)$$
MG vertex Q_i inside SG

882
883

(b)

$$r_i^M(\theta_i, \varphi_i) = r^S(\theta_i, \varphi_i)$$
MG vertex Q_i on SG surface

884
885

(c)

886   Fig. 5   Location of $Q_i'[r_i^{M\prime}(\theta_i', \varphi_i')]$ of MG with respect to SG: (a) when MG vertex Q_i outside SG,

887   (b) when MG vertex Q_i inside SG, (a) when MG vertex Q_i on SG surface

888

Fig. 6　Definition of contact point C_i for a pair of penetration points Q_i and P_i

Fig. 7　Definition of contact normal vector $\vec{n}_i$ at contact point C_i

899 **(a)**
900

901 **(c)**
902

903 **(e)**
904
905
906 Fig. 8   Definition of local overlapping volume V_i at contact point C_i: (a) whole particle view, (b)
907   local region view, (c) one-ring-neighbor vertices, (d) Example of $V_{P_i P_i^k P_i^{k+1} Q_i Q_i^k Q_i^{k+1}}$, (e) the local
908   overlapping volume V_i, (f) the top and base facets of V_i
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912

(a) (b) (c) (d)

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915
(e) (f) (g) (h)

916   Fig. 9   Packing of some example superellipsoid particles (*a*) $\eta=2.0$; (*b*) $\eta=1.25$; (*c*) $\eta=0.8$; (*d*)
917                    $\eta=0.5$; (*e*) $\zeta=0.5$; (*f*) $\zeta=0.8$; (*g*) $\zeta=1.2$; (*h*) $\zeta=1.5$
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919

(a)   **(b)**

Fig. 10   Packing density for superellipsoid (*a*) with different η and (*b*) with different ζ

(a)   **(b)**

Fig. 11   Mean coordination number Z for superellipsoid (*a*) with different η and (*b*) with different ζ

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933
934

(a)

(b)

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(c)

(d)

937
938   Fig. 12   Laboratory test of the angle of repose (*a*) container; (*b*) test step, (*c*) lift side-wall (*d*)
939   measurement of the repose angle
940
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944   (a)   (b)
945
946   Fig. 13   Illustration of (*a*) the real crushed rock for testing and (*b*) the 3D virtual model obtained by
947   the 3D laser scanner
948
949

(a)   **(b)**

Fig. 14   Numerical test of repose angle in SH-DEM: (*a*) Initial sample; (*b*) During testing

(a)   **(b)**

(c)   **(d)**

Fig. 15   Repose angles of samples with different contact friction coefficients: (*a*) contact friction = 0.1; (*b*) contact friction = 0.2; (*c*) contact friction = 0.3; (*d*) contact friction = 0.5

S1 – Sphere					
AR=1.0					
S2 – Ellipsoid					
AR=0.65					
S3 – Rocks					
AR=0.65					

Fig. 16   Ranges of shapes and the snapshots of example crushed rocks

(a)

(b)

(c)

Fig. 17   Repose angles of samples with different particle shapes: (*a*) spherical particle with AR=1.0;
(*b*) ellipsoid particle with AR=0.65; (*c*) crushed rocks with AR=0.65

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977
978   Fig. 18   Evolution of mean coordination number during repose angle tests for different samples
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984   Fig. 19   Evolution of mean rotational displacement during repose angle tests for different samples
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986
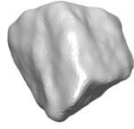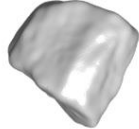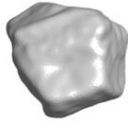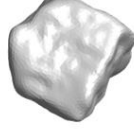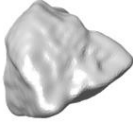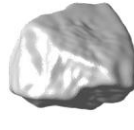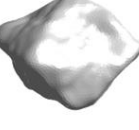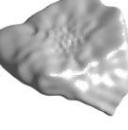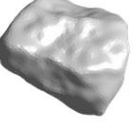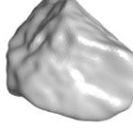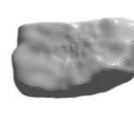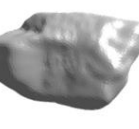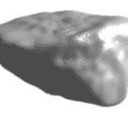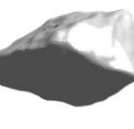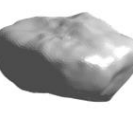
Sample 1 ——— AR=0.90~1.00					
Sample 2 ——— AR=0.75~0.85					
Sample 3 ——— AR=0.60~0.70					

Fig. 20   Ranges of shapes and the snapshots of example crushed rocks in Group C

(a)   **(b)**   **(c)**

Fig. 21   (a) non-overlapped rock aggregates; (b) consolidated rock aggregate sample; (c) Sheared
rock aggregate sample

999 **(a)**

1000 **(b)**

1001 **(c)**
1002
1003
1004 Fig. 22   Comparison of deviatoric stress between (*a*) samples of different AR; (*b*) samples of
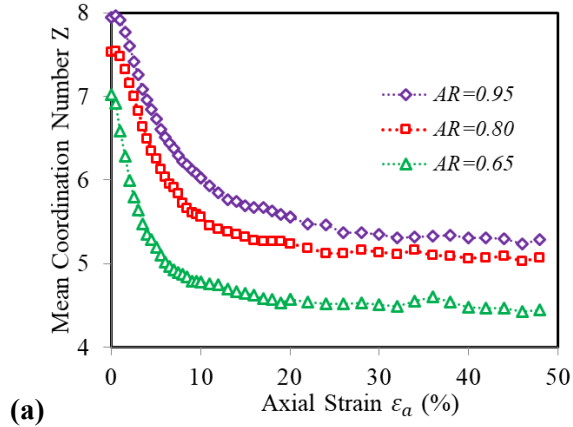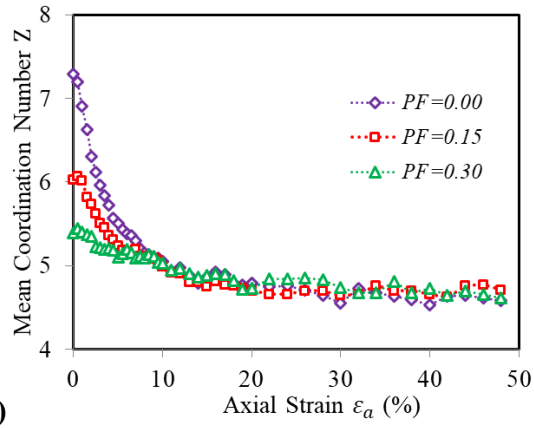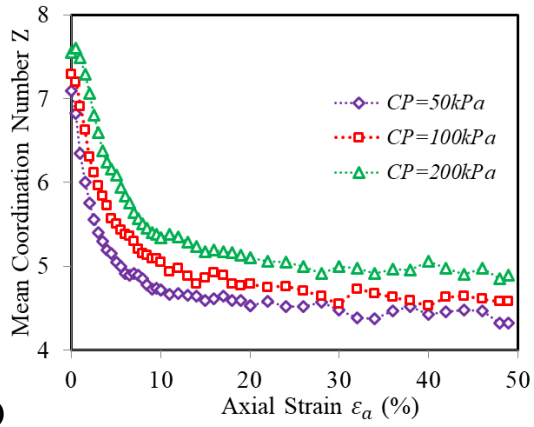1005   different preshear contact friction; (*c*) samples of different confining pressure
1006

1007 **(a)**

1008 **(b)**

1009 **(c)**

1010

1011

1012   Fig. 23   Comparison of volumetric strain between (*a*) samples of different AR; (*b*) samples of

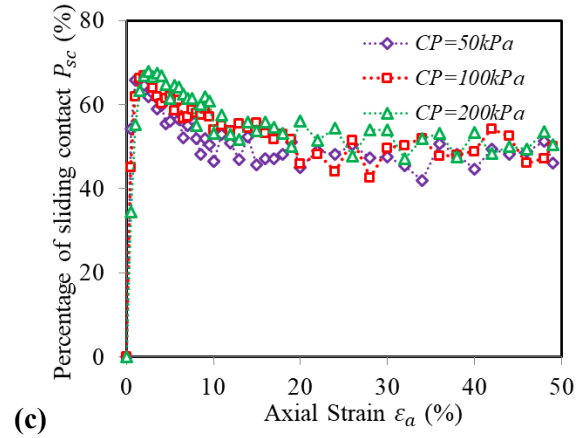1013   different preshear contact friction; (*c*) samples of different confining pressure

1014

1015 **(a)**

1016 **(b)**

1017 **(c)**

Fig. 24   Comparison of volumetric strain between (*a*) samples of different AR; (*b*) samples of different preshear contact friction; (*c*) samples of different confining pressure
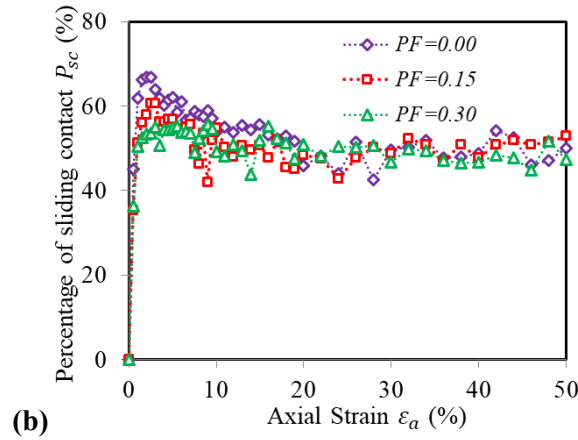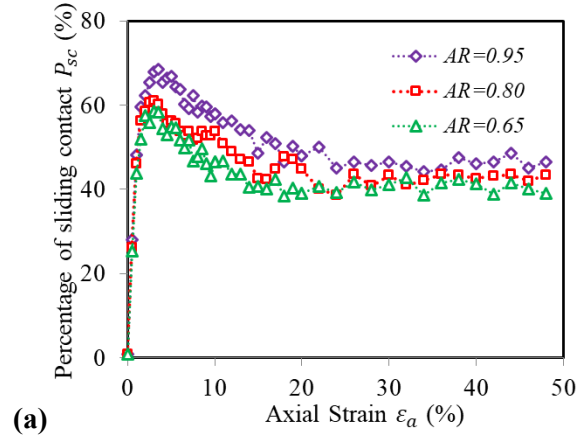
1023   **(a)**

1024   **(b)**

1025   **(c)**

1026
1027
1028   Fig. 25   Comparison of percentage of sliding contact between (*a*) samples of different AR; (*b*)
1029   samples of different preshear contact friction; (*c*) samples of different confining pressure
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1031
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