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DEM models using direct and indirect shape descriptions for Toyoura sand along monotonous loading paths

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Abstract

Two different DEM models are proposed for quantitatively simulating Toyoura sand macroscopic response along various monotonous loading paths and for a wide range of initial densities. The first model adopts spherical particles and compensates for the irregular shapes of Toyoura sand grains by adding an additional rolling resistance stiffness to the classical linear contact model. The second model follows a different strategy whereby rolling stiffness is abandoned in favor of more complex shapes in the form of a few different 3D polyhedrons defined from a 2D micrograph of Toyoura particles. After a preliminary analysis of the number of particles for optimal REV simulations, the two different modeling approaches are calibrated using triaxial compression in so-called drained conditions, adopting a common contact friction angle for the two models. Similar predictive abilities are then obtained along so-called undrained (constant volume) triaxial compression and extension paths. Although it leads to 9-times longer simulations, the polyhedral approach is easier to calibrate regarding the contact parameters. It also enables a more precise description of the microstructure in terms of particle shapes and initial fabric anisotropy, whose crucial role is evidenced in a parametric analysis.

Keywords: Toyoura sand, DEM, Rolling resistance contact model, Polyhedral particles, Anisotropy

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1 **1. Introduction**

2 As a discrete material, sand exhibits a complex behavior when subjected to
3 external loading, showing material anisotropy, non-linear stress-strain response,
4 contraction or dilation depending on the void ratio, and additional plastic strain
5 on a loading-unloading path. That mechanical behavior depends on interparticle
6 friction and on possible loss or gain of contacts between grains when sand is ex-
7 posed to an anisotropic or isotropic loading. While materials are most often sub-
8 jected to anisotropic loadings in a realistic setting, this leads to an anisotropic
9 evolution of the contact normal fabric tensor (Oda et al., 1985), whereby nor-
10 mal vectors tend to align progressively in the direction of the loading applied
11 until a constant direction is reached at the critical state (Li and Dafalias, 2012).
12 Since the Discrete Element Method (DEM) (Cundall and Strack, 1979) tracks
13 the dynamic motion of each individual particle defined in terms of mass, shape,
14 and inertia, it reproduces directly these discrete phenomena and can be used
15 as a powerful alternative technique to classical soil constitutive models (Nguyen
16 et al., 2014). Indeed, relevant macro-scale solid behaviors have been obtained
17 both qualitatively by e.g. Wang et al. (2016); Yimsiri and Soga (2010) and
18 quantitatively by Hosn et al. (2017); Lee et al. (2012); Gu et al. (2020); Rorato
19 et al. (2021) on different sands.

20 For the sake of simplicity, classical 3D-DEM simulations use spherical shaped
21 particles to represent the grains of granular materials, however, the real shapes
22 of grains are irregular and far from being that simple. For example, Miura
23 et al. (1998) presented the substantial influence of grain shape on the stress-
24 strain response of sands. Furthermore, studies on angular stainless steel powder
25 (Shinohara et al., 2000) highlighted the direct relation between particle an-
26 gularity and particle interlocking. Numerically, attempts have been made to
27 represent grain shapes inside DEM simulations starting with an additional ro-
28 tational spring at the contact level (Iwashita and Oda, 1998; Jiang et al., 2015;
29 Irazábal et al., 2017; Hosn et al., 2017; Ai et al., 2011; Sibille et al., 2019; Gu

30 et al., 2020; Rorato et al., 2021) so that it can resist relative rotation and in-
31 directly introduce the effect of the particle shapes on the DEM simulations to
32 some extent. On the other hand, clumping/overlapping a number of spheres
33 enables one to directly approximate shapes of real particles e.g. (Garcia et al.,
34 2009; Katagiri et al., 2010; Sibille et al., 2019), though with a possible negative
35 effect of the excessive roundness value for clumps on the material response. A
36 third strategy is to introduce convex polyhedral shapes inside the DEM simu-
37 lation (Lee et al., 2012; Nassauer et al., 2013). This strategy may seem to be
38 more realistic since the morphology of the grains can be reproduced correctly
39 and computational time can be optimized with an adequate number of vertices.
40 In the case where a higher number of vertices may be required, it seems inter-
41 esting to eventually resort to a level set strategy (Jerves et al., 2016; Duriez and
42 Bonelli, 2021) whereby a distance-to-surface function is considered, in a discrete
43 fashion, for every grain and contact is detected through a simple interrogation
44 of these distance data.

45 In the particular case of Toyoura sand chosen as a quite standard material for
46 geomechanics, previous DEM approaches have adopted both spherical particles
47 in conjunction with rolling resistance (Gu et al., 2020) and clump strategies
48 (Katagiri et al., 2010) for quantitative comparisons with experiments. While the
49 inclusion of clumps was somewhat beneficial, there were still some difficulties
50 in both studies for obtaining quantitative DEM results that could closely fit
51 different experiments on Toyoura sand with very different initial void ratios.

52 The present analysis aims to extend the knowledge corpus on Toyoura sand
53 and these previous DEM studies, proposing efficient and versatile DEM ap-
54 proaches for a discrete-based, quantitative simulation of that material. More
55 specifically, two 3D-DEM models are developed to simulate the mechanical be-
56 havior of Toyoura sand in porosity and loading conditions yet unexplored from a
57 quantitative point of view. The first model is a spherical grain model that incor-
58 porates rolling resistance. A second model aims to directly introduce realistic
59 shapes of Toyoura sand grains by using convex polyhedral particles. Section 2
60 describes the DEM formulations and the setup of the polyhedral and sphere

61 models while using PFC 6 software (Itasca, 2018). Section 3 presents a para-
62 metric study and calibration procedures for the two models including a brief
63 study on a proper REV definition, for an optimal setup of the 3D-DEM models.
64 Finally, Section 4 shows the validation of the two models along various stress
65 paths (drained and undrained triaxial compression and extension) and different
66 initial void ratio values.

67 **2. DEM formulations**

68 *2.1. Contact detection and resolution*

69 Every DEM cycle, contact detection and resolution schemes are applied prior
70 to the application of a constitutive contact relation. The contact detection
71 process starts with a broad phase where an axis-aligned bounding box (extended
72 cell) is generated for each particle. Contact is possible once two extended cells of
73 two pieces overlap. The second step includes a narrow phase contact detection
74 algorithm by which the pair of pieces identified as possibly colliding objects will
75 be investigated in more detail. In the case of spheres interactions, the process
76 is straightforward since it is sufficient to detect the contact by knowing the
77 position of the spheres and their radii.

78 However, in the case of polyhedrons, the process is much more complicated
79 and the Gilbert-Johnson-Keerthi (GJK) algorithm (Gilbert et al., 1988) is ex-
80 ecuted in PFC. The latter is an efficient iterative algorithm used to detect the
81 overlapping state between two convex objects. It is based on the concept of
82 the Minkowski difference of two convex polyhedrons, i.e. a convex polyhedron
83 itself which includes the origin if the two bodies overlap, while working in an
84 iterative simplex-algorithm manner to possibly avoid a full computation of that
85 difference. In order to further save computational time, the GJK algorithm is
86 applied in PFC while considering that a particle shape actually includes a core
87 polyhedron which is extended by sweeping spheres, whose common diameter is
88 given by a rounding coefficient also discussed in Section 3.2. Particles inter-
89 action is then obtained as soon as the Minkowski difference of core polygons
90 approaches the space origin within the margin of the rounding coefficient, see

91 Figure 1. The same approach can for instance be found in contact algorithms
 proposed by Zhao and Zhao (2021) for superellipsoids.

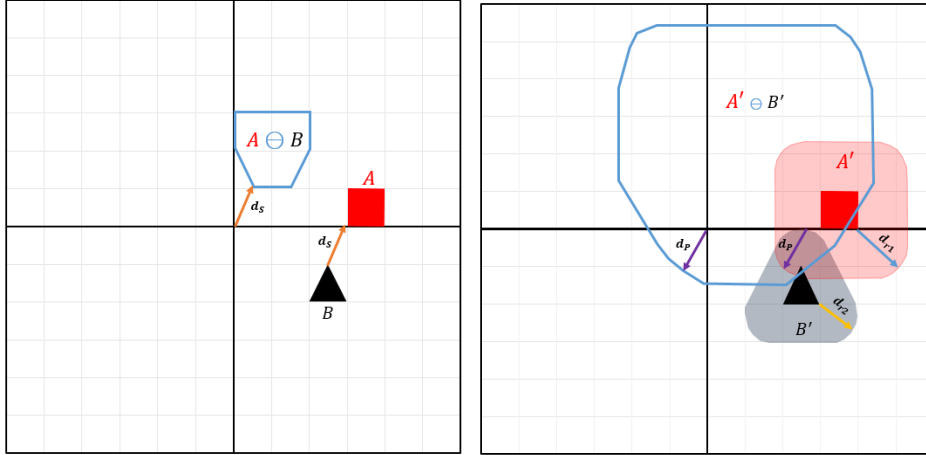


Figure 1: Contact detection and Minkowski difference for two convex particles A and B, whose core polygons do not overlap (Left) but that are still in contact due to rounding (Right, rounding artificially enlarged): 2D illustration for clarity.

92

93 Denoting $d_s > 0$ the separation length between the two core shapes as ob-
 94 tained from the Minkowski difference, $d_{r1} > 0$ and $d_{r2} > 0$ the rounding values
 95 of the two particles, a penetration depth $d_p \leq 0$ can be obtained for contacting
 96 particles as follows:

$$d_p = d_s - d_{r1} - d_{r2} \quad (1)$$

97 Contact normal is also obtained from that construction of d_p (Figure 1), while
 98 contact location is finally defined as the center of the overlapped area and de-
 99 termined based on other algorithms (Preparata and Muller, 1979; Shamos and
 100 Hoey, 1976).

101 That GJK-based determination of contact normal and penetration depth
 102 may fail depending on relative positions and rounding coefficient. In this case,
 103 the Expanding Polytope Algorithm (EPA, Bergen, 1999) is applied by PFC,
 104 with a higher computational demand.

105 In both cases, this contact resolution scheme logically affects computational
 106 times depending on the number of polyhedra vertices and those costs will be

107 estimated in Section 4.2.

108 *2.2. Inter-particle contact models*

109 Interacting particles first sustain contact forces following a classical linear
 110 contact model. An elastic normal contact force first evolves as follows:

$$111 \quad \vec{f}_n = K_n \vec{\delta}_n \quad (2)$$

$$K_n = E_{mod} \frac{\pi r^2}{R_1 + R_2} \text{ with } r = \min(R_1, R_2) \quad (3)$$

112 where $\vec{\delta}_n$ is the relative normal-displacement along the contact normal \vec{n}_c and
 113 K_n is the normal stiffness function of the normalized parameter E_{mod} and of
 114 R_1 and R_2 the radii of the two contacting spheres. The linear shear force is
 115 updated incrementally as follows:

$$\vec{f}_s = \vec{f}_s^0 + K_s \Delta \vec{\delta}_s \quad (4)$$

116 where \vec{f}_s^0 is the linear shear force at the beginning of a time step and K_s the con-
 117 tact tangential stiffness. The source of the shear displacement $\vec{\delta}_s$ is the relative
 118 tangential velocity at the contact point including the linear and angular relative
 119 velocities of the bodies. Finally, the Coulomb friction condition is imposed to
 120 limit the shear force of the contact as follows:

$$\|\vec{f}_s\| \leq \|\vec{f}_n\| \mu \quad (5)$$

121 where μ is the friction coefficient. This contact model applies to both proposed
 122 models (sphere and polyhedron).

123 In addition, a rolling resistance stiffness is also incorporated at the contact
 124 level inside the sphere model in order to compensate for the non-sphericity of
 125 the real sand particles. The contact moment is incremented linearly with the
 126 accumulated relative rotation of the contacting pieces. At the contact level the
 127 rolling stiffness and moment incremental laws are characterized as follows:

$$K_r = K_s R_m^2 \quad (6)$$

$$\frac{1}{R_m} = \frac{1}{R_1} + \frac{1}{R_2} \quad (7)$$

$$\Delta \vec{M}_r = K_r \Delta \vec{\theta}_b \quad \|\vec{M}_r\| \leq \mu_r \|\vec{f}_n\| R_m \quad (8)$$

$$\Delta \vec{\theta}_b = \Delta \vec{\theta} - \Delta \theta_t \cdot \vec{n}_c \quad (9)$$

128 Where μ_r , R_m , $\Delta \vec{\theta}$ and $\Delta \vec{\theta}_b$ are defined as the rolling friction coefficient,
 129 effective radius, rotation increment and relative bend-rotation increment, re-
 130 spectively. Equation 9 shows that for the present contact law, the twisting
 131 rotational component $\Delta \theta_t$ does not contribute to the rotational increment that
 132 is used in the rolling friction law.

133 *2.3. A 2D-image-based 3D polyhedral description of Toyoura sand grains*

134 When introducing the real grain shapes directly into DEM simulations, con-
 135 vex polyhedrons are used as 3D elements which consist of a number of vertices
 136 forming triangle facets. While the convexity of particles is an inherent limita-
 137 tion of the approach and PFC software, it will be checked it has no detrimental
 138 consequences on the results since Toyoura sand grains are measured to be close
 139 to convex by Liu and Yang (2018), with a 2D convexity = 0.937 in average while
 140 unit values would correspond to truly convex particles.

141 The definition of the present 3D polyhedral elements for Toyoura sand relies
 142 on a very simple 2D image-based workflow where a microscopic photograph of
 143 Toyoura sand is used (Fig. 2) to build three representative shapes of Toyoura
 144 sand grains, instead of the spherical grains. According to Fig. 2, Toyoura
 145 sand particles have a wide variety of shapes and different aspect-ratio values
 146 that range at least from 1.5 to 2.3, consistent with computed tomography data
 147 presented by Katagiri et al. (2010). From these observations, we propose to
 148 create just three polyhedral shapes that may reflect these morphological traits.

149 The preparation procedure is relatively simple starting from 3D PFC tem-
 150 plates of convex polyhedrons and then trying to manually adapt the vertices

151 positions to fit and mimic the form of the 2D-image of Toyoura sand. The
 152 aspect ratio is used to assess how close the proposed shapes are to the real
 153 grains. It is uniquely defined as the ratio between the largest and the middle
 154 principal dimensions: L_1/L_2 denoting $L_3 \leq L_2 \leq L_1$ the three principal di-
 155 mensions of particles. In the case of the 2D image, the information about the
 156 third (smallest) principal direction L_3 is logically missing and it is arbitrarily
 157 assumed as $L_3 = 0.75 L_2$ for the three convex polyhedrons. While there is no a
 158 prior justification for this assumption, the subsequent successful calibration and
 159 validation of the model will confirm its usefulness. In addition, the roundness
 160 of these three shapes is minimized since Toyoura sand is characterized by its
 161 sharp edges. The effect of roundness and aspect ratio on the DEM simulations
 162 will be investigated in more detail in section 3.2. Finally, the three convex
 163 polyhedrons created present different aspects and in the same time fit within
 164 the lower, middle, and upper ranges of the aspect-ratio values of Toyoura sand,
 165 as shown in Fig. 2. Indeed, Table 1 shows a high convergence between the
 166 aspect-ratio values for the proposed shapes (forming a default “Group 1”) and
 167 the real particles. An auxiliary ”Group 2” of 3 shapes is also proposed after
 168 reducing each aspect ratio i.e. the length of the larger principal dimension L_1
 169 while keeping the length of the two other principal dimensions constant, for the
 170 purpose of a parametric analysis in Section 3.

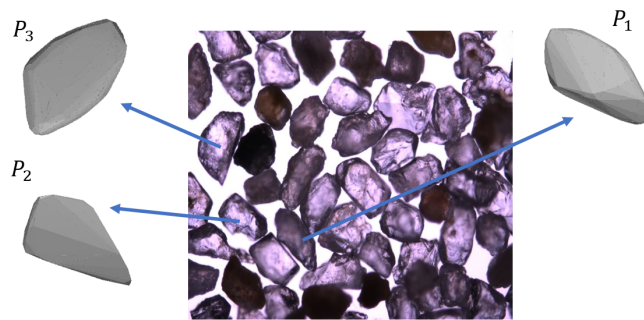


Figure 2: Original micrograph of the particle shape of Toyoura sand (Li, 2011) vs the three proposed shapes (Group 1).

171 Finally, the true sphericity shape parameter (Wadell, 1932) is also used to

Table 1: 3D-DEM polyhedra aspect-ratio vs Toyoura sand aspect-ratio

Toyourea Particle	2D-image from Fig. 2	3D-DEM Group 1	3D-DEM Group 2, see § 3.2
P_1	2.3	2.3	1.6
P_2	1.59	1.59	1.1
P_3	1.86	1.85	1.3

172 assess the shape definition of the 3D convex polyhedrons. The true sphericity
 173 parameter is defined as follows:

$$\psi = \frac{S_{Sphere}}{S_{Polyhedron}} \quad (10)$$

174 Where S_{Sphere} is the surface area of a sphere of the same volume as the particle
 175 and $S_{Polyhedron}$ is the actual surface area of the particle. Fig. 3 presents the
 176 values of the true sphericity of each particle. True sphericity values are consis-
 177 tent with those presented by Rorato et al. (2021) from computed tomography
 178 on Hostun sand, which shares a similar angularity with Toyoura sand (Altuhafi
 179 et al., 2013). Also, Fig. 3 shows that the true sphericity values of Group 1 are
 180 lower than the values of Group 2 which are aligned with the higher aspect ratio
 181 values of Group 1.

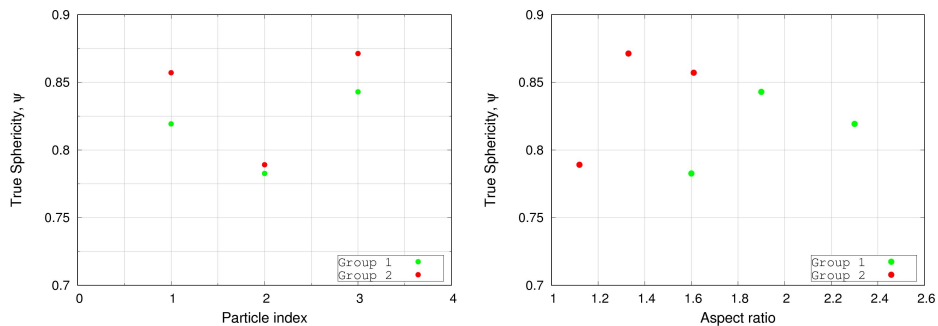


Figure 3: Left: true sphericity values of the different particles in Group 1 and Group 2. Right: Aspect ratio values vs true sphericity values for Group 1 and Group 2.

182 Finally, Table 2 presents the number of facets and vertices for each parti-
 183 cle, as directly obtained after manually adapting the templates and retaining
 184 their convex hulls for the PFC computations. In addition to computational

185 time, the obtained mechanical behavior also depends on that resolution in the
 186 shape description. A systematic study on that aspect is nevertheless outside
 187 the present scope, while the model results will serve as the sole justification for
 188 these properties.

Table 2: 3D-DEM polyhedra particles number of vertices and facets for Group 1

Particle	Number of vertices	Number of facets
P_1	128	252
P_2	78	152
P_3	203	402

189 2.4. Numerical packing and generation procedure

190 For spheres, the same particle size distribution as Toyoura sand is used in
 191 these simulations as shown in Fig. 4, modulo a scaling factor which is me-
 192 chanically transparent by virtue of the contact model, e.g. Eq. 3. Regarding
 193 the 3D-DEM polyhedral model, the ratio between the maximum and minimum
 194 convex polyhedron size is assigned for simplicity to be the same as the uni-
 195 formity coefficient C_U of Toyoura sand and equal to 1.7, as shown in Fig. 4.
 196 Size is defined for the polyhedrons based on the sphere being equivalent in vol-
 197 ume. The three representative shapes inside the generated sample share the
 198 same number of particles. Note that the present 3D-DEM approaches do not
 199 consider the particle-crushing phenomenon which would exist at high pressures
 200 (Yokura et al., 2015), while the present simulations are performed for relatively
 201 low-pressure cases (maximum confining pressure is 400 kPa).

202 Particles are enclosed within a rectangular parallelepiped with initial dimen-
 203 sions of $L_X=200$ mm, $L_Y=200$ mm, $L_Z=300$ mm and the sample is stressed
 204 using rigid walls. Unless otherwise specified, numerical samples contain around
 205 7500 particles as shown in Fig. 5 and justified in next Section 2.5.

206 The DEM microstructure is assessed by examining both the evolution of
 207 the contact normal fabric tensor and the evolution of the coordination number
 208 during the different tests. The coordination number of an assembly of particles

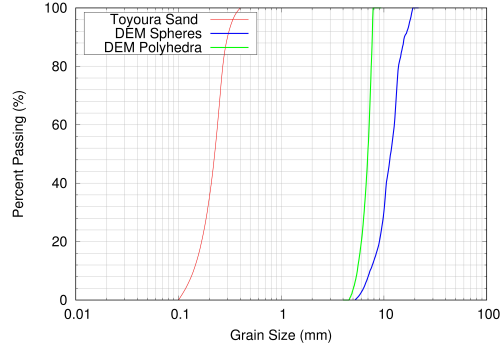


Figure 4: Particle size distributions of Toyoura sand (after Dong et al., 2016) vs DEM models.

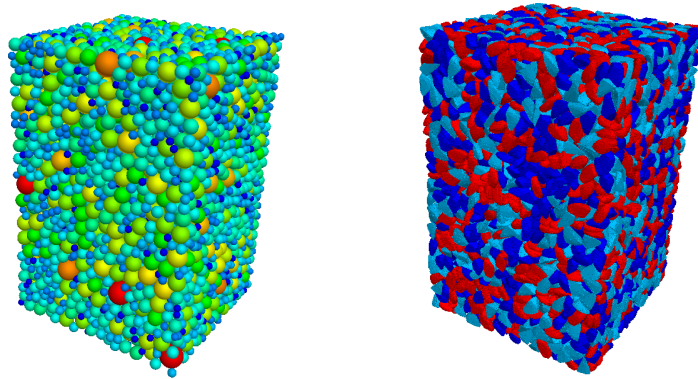


Figure 5: The two 3D-DEM models with different particle shapes: left spherical particles, where colors correspond to diameters; right convex polyhedral, where different colors correspond to different shapes (particles P_1, P_2, P_3).

209 can be expressed as follows:

$$Z = \frac{2N_c}{N_b} \quad (11)$$

210 where N_c is the number of contacts and N_b is the number of bodies. The contact
211 normal fabric tensor F_{ij} can be evaluated as follows:

$$F_{ij} = \frac{1}{N_c} \sum_{cont.} n_i \otimes n_j \quad (12)$$

212 where n_i is the contact normal direction. The anisotropy A of the fabric tensor
213 F_{ij} is quantified and defined as the ratio between the deviatoric part of the
214 fabric tensor and one-third of the first invariant of the fabric tensor. By taking
215 into account the axisymmetric condition of the triaxial test around axis Z , the
216 equation yields to:

$$A = \frac{3(F_{ZZ} - F_{XX})}{F_{ZZ} + 2F_{XX}} = 3(F_{ZZ} - F_{XX}) \Rightarrow |A| = 3(F_I - F_{III}) \quad (13)$$

217 Where F_I and $F_{III} = F_{II}$ are the fabric eigenvalues.

218 Inspired by laboratory tests where samples could be prepared by using dif-
219 ferent methods such as air pluviation (Tatsuoka et al., 1986) or moist tamp-
220 ing (Verdugo and Ishihara, 1996) with an influence on initial fabric, two different
221 procedures are herein adopted for packing generation.

222 As a first option, DEM samples are prepared starting from a cloud of parti-
223 cles with no contacts. Afterwards, an isotropic compaction is applied by moving
224 the walls towards the sample with maximum velocity and target compaction
225 pressure. During the compaction phase, porosity can be controlled depending
226 on the friction coefficient and rolling coefficient (for the spherical cases) values
227 which are tuned, independently of the subsequent shear loading phase, to reach
228 the same initial porosity values as the reference experiments considered below.

229 In a second preparation method, the cloud of non-overlapping particles is
230 first let to settle under vertical acceleration (enhanced gravity). A top wall then
231 moves downwards to ensure good contact with the particles before applying an
232 isotropic pressure by moving the six walls towards the sample, until forming the
233 consolidated stage of the triaxial loading.

234 The spherical model is observed to be insensitive to the preparation proce-
235 dure for what concerns its fabric, which can be explained by the isotropic nature
236 of spherical shapes, presented simulations with spheres then apply indistinctly
237 to either preparation method and start with a fairly isotropic fabric. On the
238 other hand, the polyhedron model shows a strong sensitivity to the prepara-
239 tion method, which will be discussed in connection with contact parameters in
240 Section 3.3.

241 Finally, the quasi-static condition is ensured for the different triaxial tests
242 by satisfying the following condition for the inertial number $I_r \leq 10^{-4}$.

243 *2.5. Effect of the number of particles on 3D REV response*

244 Because the DEM results are here classically interpreted in average through
245 the consideration of stresses, strains or fabric tensor defined at the sample scale,
246 it is important to check whether a Representative Elementary Volume (REV)
247 is reached in the sense that the mechanical response is fully defined from the
248 average initial properties (e.g. porosity) with no other influences coming e.g.
249 from the placements of individual particles in each case. For given average initial
250 properties, a previous study (Chareyre, 2003) illustrated how results dispersion
251 (e.g. on peak values or volumetric response) possibly exists but decreases when
252 the number of particles increases towards forming a REV. Previous 3D-DEM
253 studies at the REV scale can be found with various numbers of particles, possibly
254 as different as 1000 (Cheng et al., 2018) and about 44000 (Gu et al., 2020). A
255 REV determination is then proposed in this study for the spherical model,
256 investigating the effect of the number of particles on the homogeneity of the
257 REV and its impact on the computational time, while keeping all the other
258 parameters of the DEM simulation constant (Table 3). The number N of spheres
259 in the sample is changed gradually from 400 to 14500 spheres, using smaller
260 spheres and a constant total size of the sample since the present DEM results
261 are particle size-independent.

262 To obtain a view inside the different samples, the porosity was monitored in
263 two different ways. A first measure calculated the overall porosity n_b based on

Table 3: Spherical DEM parameters

Remark	Contact				Packing (see also Fig. 4 for psd)		
	E_{mod} (MPa)	K_n/K_s (-)	μ (-)	μ_r (-)	N_b (-)	Initial n_b (-)	Initial A (-)
REV analysis of Section 2.5	450	3	0.6	0.38	from 400 to 14500	0.402	0
Rolling resistance analysis of Section 3.1	450	3	0.6	0 or 0.38	7530	0.400	0
Proposed model for Toyoura sand (Sections 3.4 and 4)	450	3	0.6	0.38	7530	from 0.40 to 0.453	0

264 Eq. 14, representing the average porosity for the whole sample.

$$n_b = 1 - \frac{1}{L_x L_y L_z} \sum_{N_b} V_b \quad (14)$$

265 where N_b is the total number of (spherical) particles inside the sample and V_b
266 is the volume of one ball. A second value of the porosity n_c is more local, being
267 defined within a measurement region, as described in Eq. 15.

$$n_c = 1 - \frac{\sum_{N_b} V_b + \sum_{N_i} V_i - \sum_{b_c} V_c}{V_{reg}} \quad (15)$$

268 where V_i is the intersected volume between balls and the measurement region,
269 N_i is the number of balls that intersect the measurement region and V_c is the
270 overlapped volume between the balls that lie inside the measurement region.
271 Here, the measurement region is a ball positioned at the center of the sample
272 and has a diameter equal to 90 % of the shortest length of the sample. Thus, the
273 homogeneity of the sample in terms of porosity can be evaluated by comparing
274 the two calculated porosities mentioned previously.

275 Doing so, global porosity n_b is controlled to be equal to 0.402 for 9 samples
276 with different numbers of particles, while the second value of the porosity n_c is
277 locally evaluated for each sample. The results illustrated in Fig. 6 show that
278 by increasing the number of particles, the sample becomes more homogeneous
279 thanks to a smaller proportion of particles along boundaries and the values of
280 the two calculated porosities become closer. On the other hand, for the samples

281 that use lower numbers of particles, voids are concentrated at the volume that
 282 is adjacent to the peripheral walls. Fig. 6 also shows how computational time
 283 increases by increasing the number of particles used in the simulation. Com-
 284 putational times refer to a parallel execution of PFC on a workstation with 8
 285 cores, 3.0 GHz CPU with 64 GB RAM. Finally, Fig. 7 shows that the effect
 286 of the number of particles on the deviatoric and volumetric responses becomes
 287 negligible starting from a number of particles N equal to 7500, defining the REV
 288 scale consistently with e.g. Duverger et al. (2021) on another granular material.

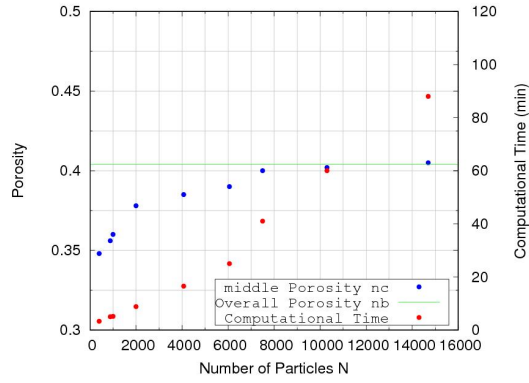


Figure 6: Number of spheres N vs computational time and n_c, n_b .

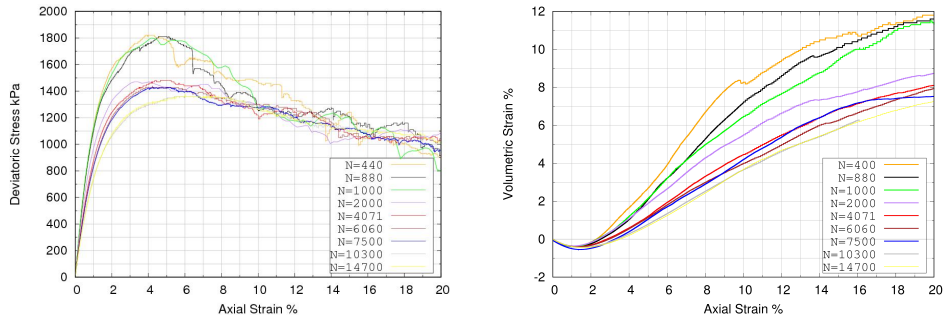


Figure 7: Effect of the number of particles on the deviatoric and volumetric responses for the same initial porosity $n_b=0.402$ and confining pressure = 400kPa.

289 **3. Parametric analysis and calibration of the spheres and polyhedron**
 290 **models**

291 An extended parametric study was performed on the sphere and polyhedron
 292 models. Concerning the sphere model, the study contained the effect of the
 293 presence or absence of the rolling resistance stiffness, see Table 3. For the
 294 polyhedron model, the study involved the effect of the shape parameters: aspect
 295 ratio or true sphericity, roundness, as well as the effect of the initial anisotropy
 296 value in conjunction with contact parameters. Table 4 presents a summary of
 297 the proposed simulations for the polyhedron model.

Table 4: Summary of simulations with the 3D-DEM polyhedron model

Object	Set number (from Table 5)	Polyhedrons Group (from Table 1)	Variable condition(s)
Influence of shape parameters in Section 3.2	Set 1	Group 1	Particles relative rounding [0.0001,0.01,0,5]
Influence of shape parameters in Section 3.2	Set 1	Group 1 vs Group 2	Particles aspect ratio (i.e. true sphericity)
Interplay of initial fabric with contact parameters in Section 3.3	Set 1 vs Set 2	Group 1	Sample preparation (i.e. initial fabric A) and contact parameters
Proposed model for Toyoura sand in Sections 3.4 and 4.1	Set 2	Group 1	Void ratios, confining pressures and loading paths

298 *3.1. Influence of rolling resistance on the sphere model*

299 The effect of the rolling resistance coefficient μ_r is investigated herein. Fig. 8
 300 shows the results of DEM simulations with and without μ_r together with the
 301 corresponding experimental data for a drained triaxial test for Toyoura sand
 302 obtained by Fukushima and Tatsuoka (1984). Fig. 8 shows the advantage that
 303 can be added by the rolling resistance friction law to the strength and volumetric
 304 strain behaviors for the sphere model. In addition, the simulations confirm
 305 the crucial role played by the rolling stiffness to represent the irregular-shaped
 306 particles of Toyoura sand indirectly.

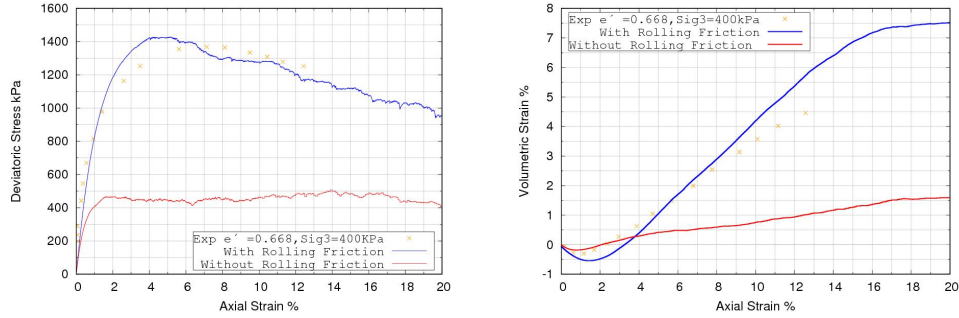


Figure 8: Effect of the rolling resistance friction on the DEM results in comparison to experimental data by Fukushima and Tatsuoka (1984). Initial void ratio=0.668 and confining pressure=400kPa

3.2. Influence of shape parameters for the polyhedral grain model

The roundness of the particle plays an important role on the mechanical response (Cho et al., 2006) so that a parametric study is carried out on the effect of the particles' roundness when using polyhedrons, through the consideration of the sweeping spheres and their rounding coefficient primarily used for the contact algorithm discussed in Section 2.1. A relative rounding coefficient for sweeping spheres of radius r_1 is defined in PFC as the ratio between r_1 and the radius r_2 of another sphere that has the same volume as the polyhedron. Fig. 9 presents three final shapes for the same initial polyhedrons P_1 , P_2 and P_3 after rounding their core shapes using different relative rounding values. The simulations were performed by using the contact parameters of Set 1 (Table 5) and by using the polyhedral shapes from Group 1 (Table 1).

Table 5: 3D-DEM polyhedron model parameters

Set	Contact			Packing (see also Fig. 4 for psd)		
Number	E_{mod} (MPa)	K_n/K_s (-)	μ (-)	N_b (-)	Initial A (-)	Relative rounding (-)
Set 1	300	2	0.8	7490	-0.20	0.0001
Set 2	200	3	0.6	7490	0.26	0.0001

Fig. 10 and 11 illustrate the effect of the rounding of the particles on the macroscopic and microscopic behaviors. The initial coordination number increases by decreasing the rounding of the particles. Accordingly, the sample

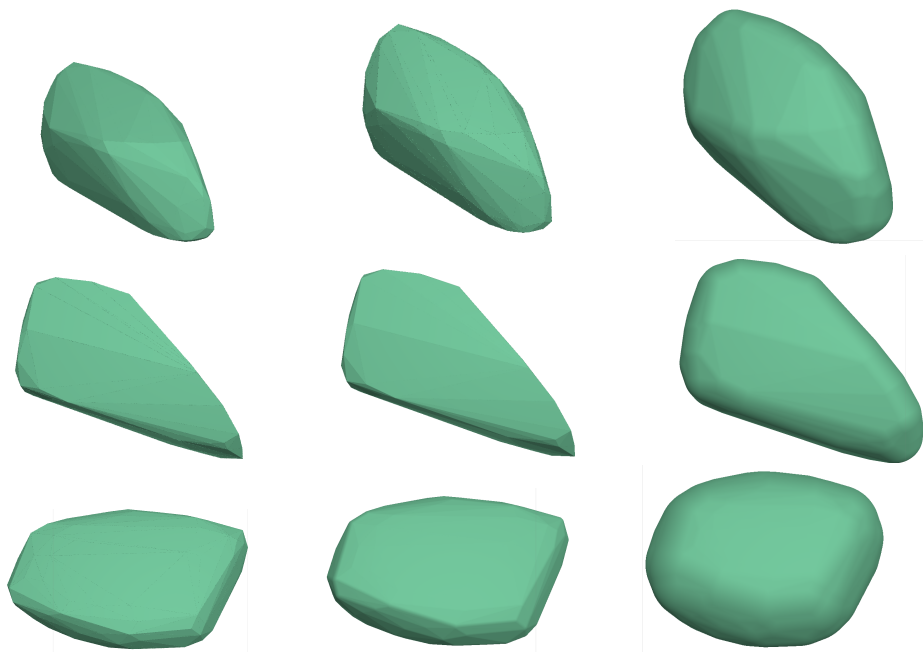


Figure 9: Different relative rounding values for particles P1 (top row), P2 (middle row) and P3 (bottom row). The particles have relative rounding values from left to right 0.0001, 0.01 and 0.5.

322 with a lower rounding value has a higher resistance and a larger volumetric
 323 dilation. Fig. 11 shows the evolution of the anisotropy of the contact normal
 324 fabric tensor, as per Eq. 13, during the shearing phase for various roundness
 325 values. Note that the initial anisotropy observed in the case of the polyhedron
 326 model is due to the non-spherical shapes of the polyhedron (Azéma and Radjai,
 327 2010). The results show that the sample with a higher relative rounding value
 328 has less tendency to present an initially anisotropic fabric tensor. Finally, since
 329 Toyoura sand is observed to be the less rounded among various sands from 2D
 330 images (Liu and Yang, 2018), therefore the relative rounding value of 0.0001 is
 331 used for the calibration of the polyhedron model in Section 3.4.

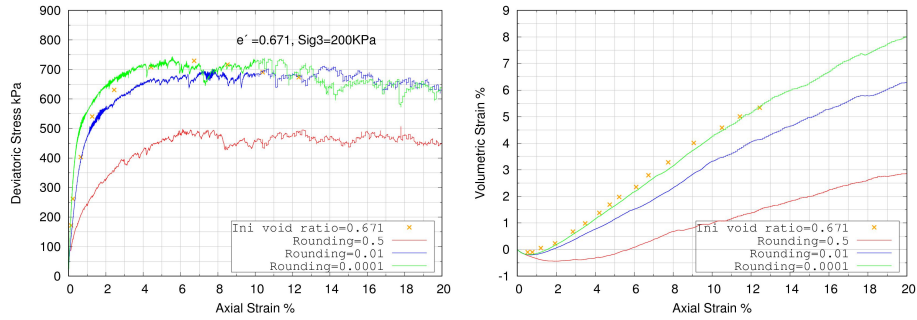


Figure 10: Evolution of deviatoric stress vs axial strain (left) and volumetric strain vs axial strain (right) for different relative rounding values. Cross points are experimental data by Fukushima and Tatsuoka (1984).

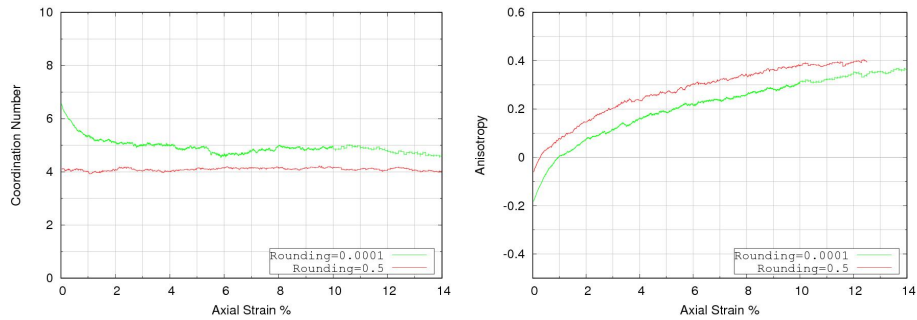


Figure 11: Evolution of the fabric tensor and coordination number vs axial strain during the drained triaxial test for different relative rounding values with a mean effective stress = 200 kPa and initial void ratio = 0.671.

332 Next, the effect of the particle aspect ratio is investigated by considering the
333 Group 2 shapes with a reduced aspect ratio (Table 1) together with those of
334 Group 1 while keeping all the other parameters constant (set 1 of Table 5). The
335 results in Fig. 12 show the crucial role played by the particle aspect-ratio on the
336 strength of granular material. The sample with higher aspect-ratio values, or
337 lower values for true sphericity, has a higher resistance and a larger volumetric
338 dilation. In addition, Fig. 13 presents the evolution of the fabric tensor and
339 coordination number for the two groups during the triaxial compression test.
340 The results show that the sample with particles of Group 2 (lower aspect-ratio
341 value) has less tendency to induce an initially anisotropic fabric and lower initial
342 coordination number.

343 The above results about the dependency of the initial anisotropy values on
344 the aspect ratio and rounding values are consistent with the results of the spheres
345 model (isotropic well-rounded particles) presented in Fig. 14 which show that
346 the anisotropy value is almost equal to zero after the confining phase of the
347 triaxial test.

348 *3.3. Interplay of initial fabric with contact parameters for the polyhedron model*

349 Unlike spheres, polyhedron packings show different initial fabric anisotropy
350 depending on the generation procedure. Using the first method exposed in Sec-
351 tion 2.4 (isotropic compaction), an initial anisotropy is obtained because of the
352 irregular shapes which make the fabric more sensitive to be initially anisotropic,
353 with $A = -0.2$ here. In the second method involving vertical settlement, pack-
354 ing shows an anisotropy value $A = 0.26$ which means that the contacts were
355 more aligned vertically. It is worth mentioning that X-ray tomography of labo-
356 ratory sand samples prepared by air pluviation method (Wiebicke et al., 2020)
357 confirm the present DEM observations in two aspects. First, Wiebicke et al.
358 (2020) observed a rounded Caicos sand to show an isotropic fabric even after
359 pluviation, consistent with our previous observations on spheres. Second, they
360 also measured after preparation an initially anisotropic fabric, with virtually
361 the same A , on Hostun sand which shares similar shape features with Toyoura

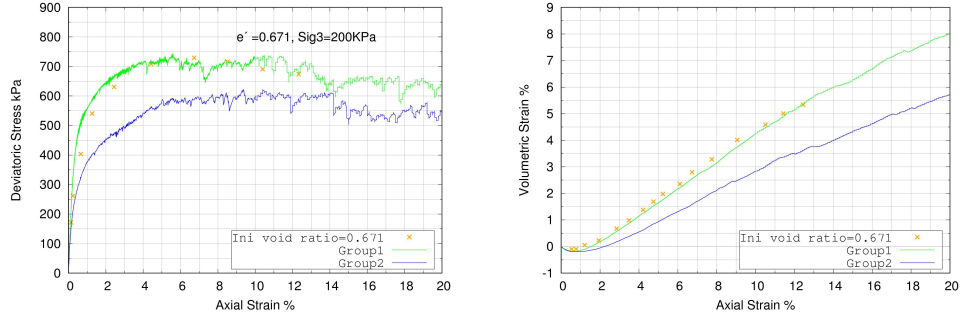


Figure 12: Evolution of deviatoric strain vs axial strain and volumetric strain vs axial strain for different aspect-ratio values. Cross points are experimental data (Fukushima and Tatsuoka, 1984).

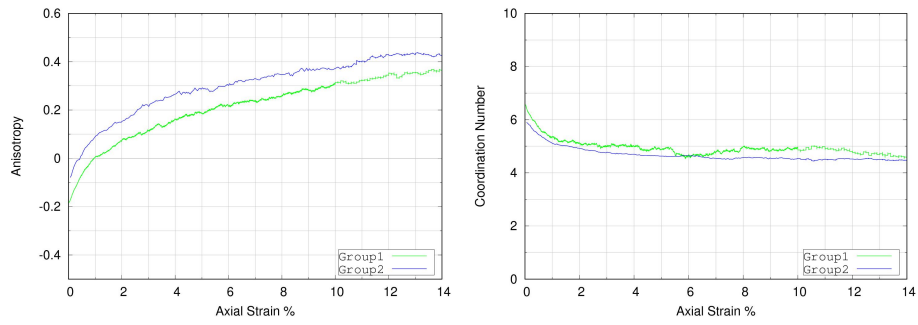


Figure 13: Evolution of the fabric tensor and coordination number vs axial strain during the drained triaxial test for different aspect-ratio values with a mean effective stress = 200 kPa and initial void ratio = 0.671.

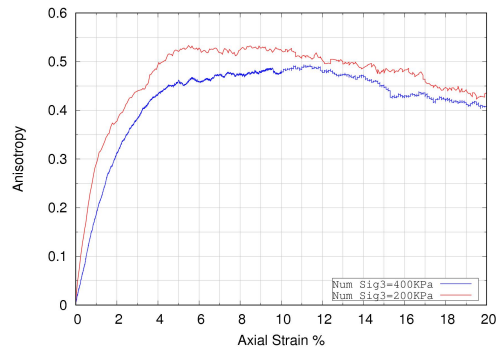


Figure 14: Evolution of the fabric anisotropy A of the sphere model during two drained triaxial tests with confining pressures = 200, 400 kPa and initial void ratios = 0.671, 0.668.

362 sand according to Altuhafi et al. (2013).

363 Aiming for an equivalent calibration exercise in spite of the different fabrics,
 364 both samples can still reproduce a given drained triaxial compression (Fig. 15),
 365 by using two different sets of parameters (Set 1 or 2 in Table 5). Because the
 366 Set 1 sample with initial $A = -0.2$ shows more contact normal vectors aligned
 367 to the horizontal (X, Y) plane than to the vertical direction Z which is the
 368 major principal direction for the test, it is necessary to adopt higher contact
 369 parameters in Set 1: $(E_{mod}; \mu) = (300 \text{ MPa}; 0.8)$ instead of $(200 \text{ MPa}; 0.6)$ for
 370 Set 2.

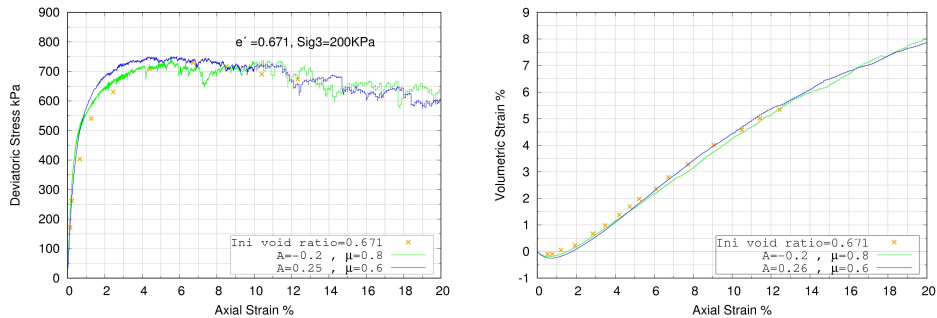


Figure 15: Two possible calibrations of the polyhedron model on a drained triaxial test by (Fukushima and Tatsuoka, 1984) by using two different sets of contact parameters in connection with two different preparation methods, i.e. fabric: Set 1 (e.g. $\mu=0.8$ while $A = -0.2$) and Set 2 (e.g. $\mu=0.6$ while $A = 0.26$)

371 The predictive performances of these two polyhedron models are then compared
 372 on different stress paths such as undrained triaxial compression and extension.
 373 Fig. 16 shows simulations of Set 1 and Set 2 for triaxial compression and extension
 374 tests at the same initial mean effective stress (400 kPa) along with experimental data
 375 of dry-deposited Toyoura sand from Yoshimine (2013).
 376 When performing such blind predictions, the model with Set 1 parameters can
 377 successfully fit the undrained triaxial compression but its behavior is much too
 378 stiff when sheared in extension. However, the model with Set 2 parameters gives
 379 a very good prediction for both the compression and extension paths in terms
 380 of deviatoric and effective mean pressure responses, as shown in Fig. 16.

381 These simulations highlight how DEM models may appear to show non-

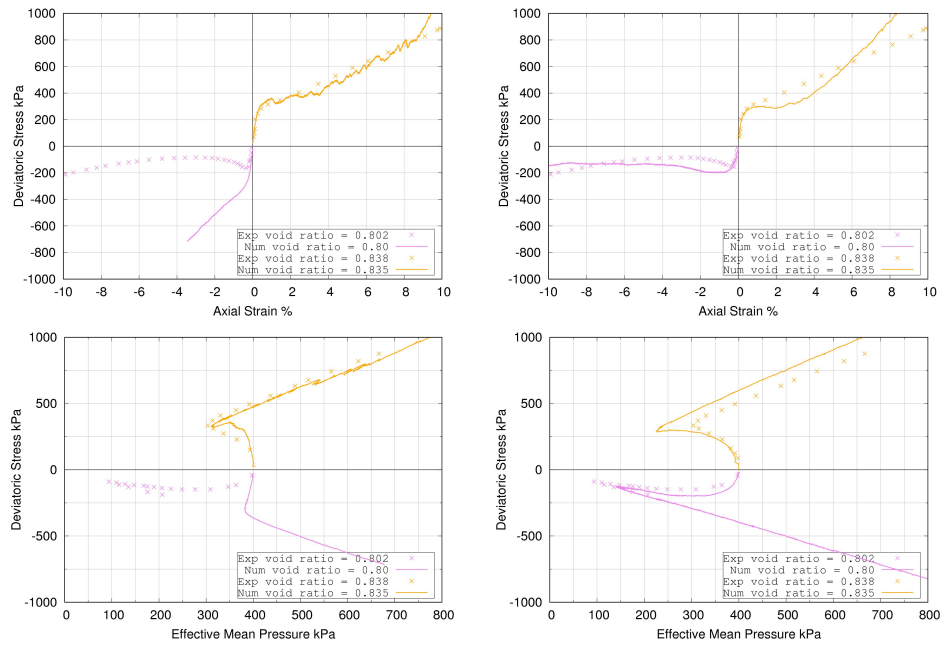


Figure 16: Predictions of two polyhedron models along undrained compression and extension stress paths against experimental data by Yoshimine (2013): interplay of packing anisotropy and contact parameters. Left: Set 1 model with $A=-0.2$ and e.g. $\mu=0.8$; right: Set 2 model with $A= 0.26$ and e.g. $\mu=0.6$

382 unique contact parameters or fail in their predictions, if one considers a limited
383 set of loading paths or neglects fabric considerations. Here, the second prepa-
384 ration procedure (vertical deposition under gravity) associated with Set 2 is
385 more similar to laboratory preparation methods (the air pluviation method)
386 and gives a more physical fabric, with contact normal vectors that tend to align
387 along the direction of deposition. It then enables the DEM model to be more
388 performant along various loading paths, as it will be further evidenced in the
389 coming sections.

390 *3.4. Calibrated parameters*

391 Final calibration of both spherical (with four contact parameters, Table 3)
392 and polyhedron (with three contact parameters, Table 5) models is finally pro-
393 posed, based on a drained triaxial compression test for Toyoura sand obtained
394 by Fukushima and Tatsuoka (1984) and presented in Woo and Salgado (2015).
395 The sphere model is calibrated for an initial void ratio and a confining pressure
396 equal to 0.668 and 400kPa respectively, while the polyhedron model considers
397 an initial void ratio and confining pressure equal to 0.671 and 200 kPa respec-
398 tively. Other tests will be considered for validation in Section 4.1, such that
399 both models will eventually address the same experimental data set, either in a
400 calibration or in a validation stage. It is also recalled that the DEM models have
401 initial void ratio values equal to the experimental void ratios for the different
402 triaxial tests, see Section 2.4.

403 Following Sections 3.2 3.3, the polyhedron model adopts particles with Group
404 1 shapes and the Set 2 configuration in Table 5 because laboratory samples were
405 prepared using the air pluviation method.

406 The calibration results of both models can closely fit the experimental data
407 as shown in Fig. 17. It is remarkable that the friction coefficient is the same in
408 both DEM approaches, highlighting the role of the rolling resistance model to
409 take into account complex particle shapes in an indirect way.

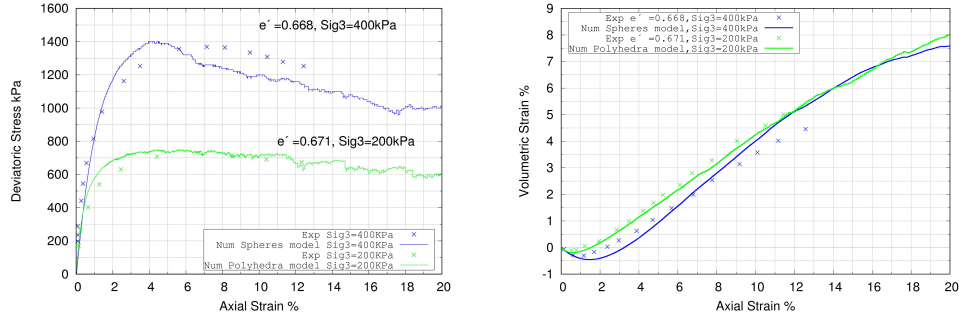


Figure 17: Calibration of the sphere and polyhedron models by using one drained triaxial test in each case. The cross points are experimental data (Fukushima and Tatsuoaka, 1984).

410 4. Validation of the sphere and polyhedron models and discussion

411 4.1. Validation

412 The two models were finally validated checking their prediction abilities for
 413 other drained triaxial tests and for undrained conditions.

414 Fig. 18 and 19 represent the predictions of sphere and polyhedron models
 415 together with the experimental results for the drained triaxial tests for various
 416 initial void ratios and confining pressures. The results of the two models present
 417 a good fit with the corresponding experimental results for the deviatoric stress
 418 and volumetric strain responses. A slight difference is just to note for the
 419 volumetric strain behavior in the case of the two relatively loose (less dilatant)
 420 samples. We observed in other simulations with spheres, not presented here,
 421 that introducing a flexible membrane boundary condition instead of rigid walls
 422 would slightly improve the agreement for these two tests.

423 As for the undrained compression tests, a fully strain-controlled model with
 424 constant volume is used to simulate such a loading condition. Simulations are
 425 reported for extension and compression conditions and for six samples with dif-
 426 ferent initial void ratio values which ranged between 0.794 and 0.88 and could
 427 be obtained systematically in the simulations. The simulated responses agree
 428 closely with the experimental data, revealing the good capability of the pro-
 429 posed models to capture the complex behavior of the granular material during
 430 the undrained conditions, as shown in Fig. 20 and 21. Firstly, the behavior

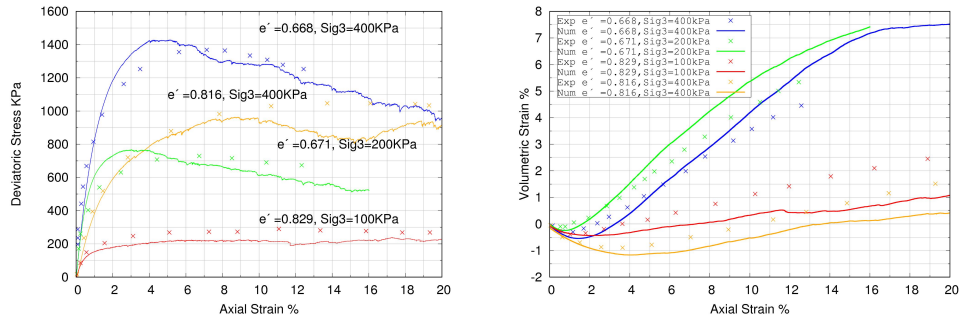


Figure 18: Behavior of the sphere model for Toyoura sand under various drained triaxial compressions serving as calibration ($e_0 = 0.668; \sigma_3 = 400$ kPa) and validation paths. Experimental data from (Fukushima and Tatsuoka, 1984)

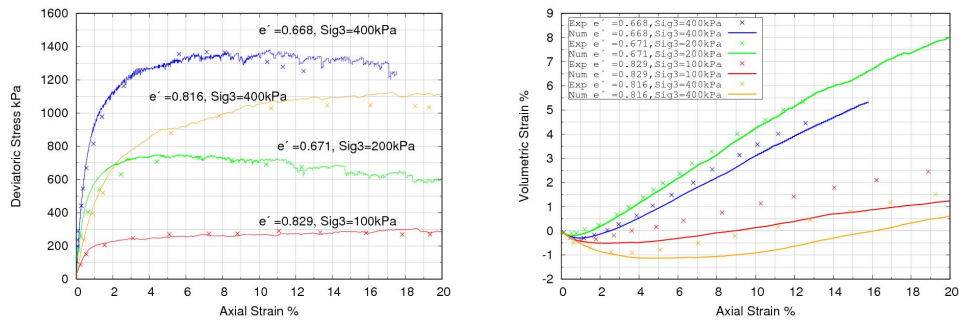


Figure 19: Behavior of the polyhedron model for Toyoura sand along various drained triaxial compressions serving as calibration ($e_0 = 0.671; \sigma_3 = 200$ kPa) and validation paths. Experimental data from (Fukushima and Tatsuoka, 1984)

431 is sensitive to different initial void ratios. Secondly, the model captures the
 432 difference between the extension and compression triaxial behaviors naturally,
 433 confirming the fact that the sand response is much more contractive in triaxial
 434 extension than when loaded in triaxial compression.

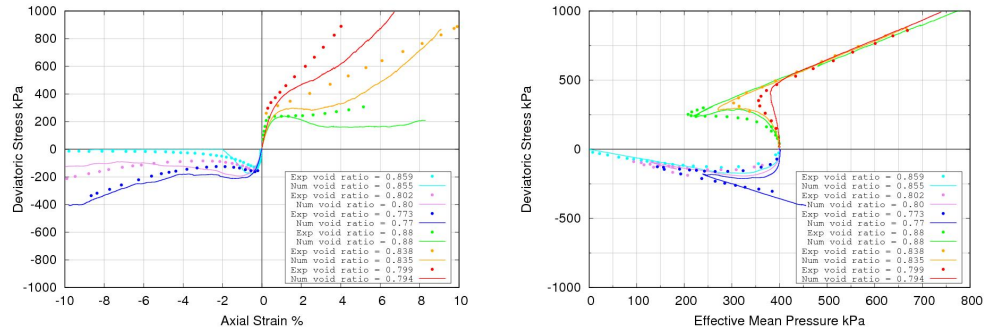


Figure 20: Validation of sphere model for Toyoura sand sheared under undrained triaxial extension and compression for various void ratios and an initial mean effective pressure = 400 kPa. Experimental data by (Yoshimine, 2013).

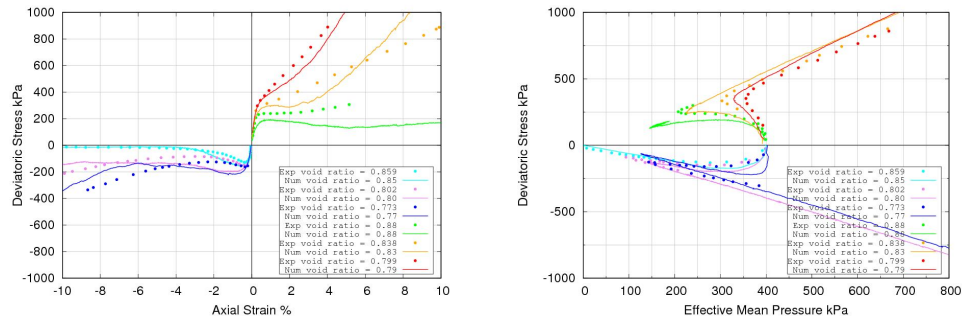


Figure 21: Validation of the polyhedral grain model for Toyoura sand under undrained triaxial extension and compression for various void ratios and an initial mean effective pressure = 400 kPa. Experimental data by (Yoshimine, 2013).

435 *4.2. Discussion*

436 While the two models give very good predictions for the macroscopic me-
 437 chanical behavior of Toyoura sand, the polyhedron model showed a somewhat
 438 higher capability of fitting the volumetric strain behavior and especially the
 439 initial contraction regime and substantial differences remain from a microscopic

440 point of view. For example, for the same initial void ratios, the 3D-DEM polyhe-
441 dron model has an initial coordination number higher than the 3D-DEM model
442 with the rolling resistance model, as shown in Fig. 22.

443 Furthermore, since the polyhedral model contained flat and angular-shaped
444 particles, the sample showed an inherent anisotropy, which is a function of
445 the generation procedure. This feature was reported in previous studies of
446 Toyoura sand (Yoshimine et al., 1998; Tatsuoka et al., 1986) and could not be
447 captured by using spherical particles. While this has not been detrimental to
448 the performances of the spherical model in the present study on monotonous
449 paths, some unrealistic fabric for spheres model has been reported by Zhao et al.
450 (2018), which may relate with lower predictions abilities of these approaches in
451 some cases, such as cyclic undrained triaxial test (Gu et al., 2020; Sibille et al.,
452 2021).

453 On practical aspects, the simulations using the polyhedral particles are still
454 a time-consuming task, with the calculation time depending on the number of
455 vertices of each piece utilized inside the contact detection scheme. Fig. 22 shows
456 that the computational time of the present 3D-DEM polyhedron model was al-
457 most 9 times higher than the 3D-DEM model with a rolling resistance model
458 and for the same numerical conditions. However, the rolling resistance contact
459 model includes four contact mechanical parameters which are somewhat tedious
460 to calibrate, while only three such parameters are required for the polyhedron
461 model. While some complexity hides in the latter model behind the character-
462 ization of the representative shapes, experimental techniques are getting more
463 and more available for a direct measurement of those shapes (e.g. Katagiri et al.,
464 2010; Rorato et al., 2021).

465 **5. Conclusions**

466 This paper has established two discrete element models with different kinds
467 of rigid particles for describing the microscopic and macroscopic behaviors of
468 Toyoura sand, as well as a thorough study on important model features from
469 the particle- to the packing-scale.

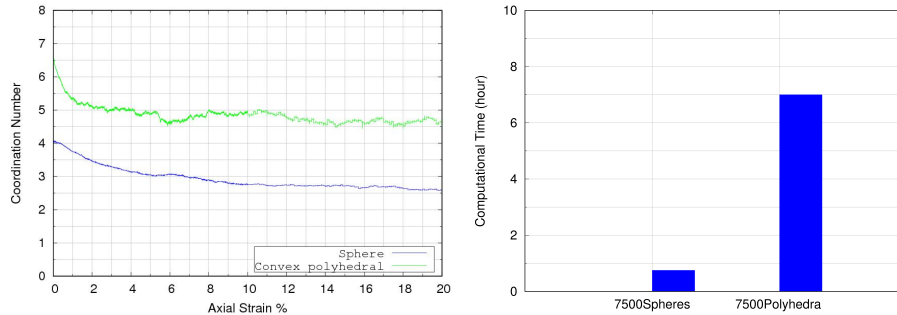


Figure 22: Left: evolution of the coordination number for the sphere model and convex polyhedron model during drained triaxial test with an initial porosity $n=0.402$. Right: computation time for two drained triaxial tests for the two models with a target axial strain = 0.2.

470 At the particle scale, the crucial role of shapes, roughnesses and angularity
 471 of Toyoura sand grains on its mechanical response was taken into account within
 472 the 3D-DEM simulations, either artificially by adding rolling resistance stiffness
 473 between spherical particles or by introducing the realistic particles via convex
 474 polyhedron shapes. The convex polyhedron model was an image-based model
 475 in which the 2D shape and the aspect-ratio of three different real particles of
 476 Toyoura sand were used to create three representative particles for Toyoura
 477 sand that shared the same number of particles inside the 3D-DEM model. For
 478 a better control over the shapes proposed, a parametric study was carried out
 479 on the effect of the particles' roundness and aspect ratio on the mechanical
 480 response. The results first showed that samples with a lower aspect ratio and
 481 a higher roundness value have less tendency to be initially anisotropic after an
 482 isotropic packing preparation. Second, the strength of the sample increased
 483 with an increasing particle aspect ratio and a decreasing roundness, along with
 484 a more dilatant volumetric response.

485 At the packing-scale, the REV configuration in terms of the number of par-
 486 ticles is the first important issue. As for the optimization of a 3D-DEM simu-
 487 lation, 7500 particles were chosen to construct a homogeneous sample in terms
 488 of porosity, showing a unique stress-strain behavior. Moreover, a study on the
 489 effect of the initial fabric on triaxial compression and extension tests empha-

490 sized once more the crucial role played by the initial contact normal orientation
491 on the mechanical response. This parameter corresponded to different sample
492 preparation methods for the laboratory triaxial tests. Having a sample that
493 was prepared in the same way as the experimental laboratory sample, allowed
494 us to select one set of parameters capable of calibrating and validating different
495 stress paths. The numerical simulations of the two models of Toyoura sand
496 proposed showed remarkable quantitative and qualitative agreement with the
497 experimental results for various stress paths and a wide range of initial void
498 ratios.

499 Finally, the computational time for the convex polyhedron model was found
500 to be nine times higher than that of the sphere model using the same numerical
501 conditions such as the number of particles, strain rate and final axial strain
502 value.

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507 support and for providing PFC software.

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