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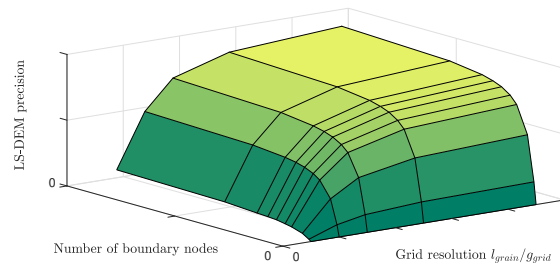
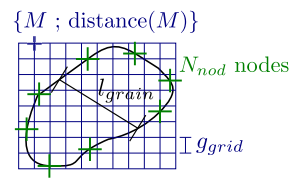
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Graphical Abstract

Precision and computational costs of Level Set-Discrete Element Method (LS-DEM) with respect to DEM

J. Duriez, S. Bonelli



Precision and computational costs of Level Set-Discrete Element Method (LS-DEM) with respect to DEM

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Abstract

The Level Set-Discrete Element Method (LS-DEM) extends DEM towards arbitrary grain shapes by storing distance-to-surface values on a grid for each Discrete Element (DE), together with considering boundary nodes located onto the DE's surface. Both these ingredients are shown to affect the precision and computational costs of LS-DEM, considering various numerical simulations at the contact- and packing-scales for ideal spherical and superellipsoid shapes. In the case of a triaxial compression for spherical particles, approaching with a reasonable precision the reference result obtained in classical DEM requires the grid spacing to be smaller than one tenth of particle size, as well as using a couple thousands of boundary nodes. Computational costs in terms of memory (RAM) or evaluation time then increase in LS-DEM by two or three orders of magnitude. Simple OpenMP parallel simulations nevertheless significantly reduce the increase in time cost, possibly dividing the latter by 20.

Keywords: computational cost, particle shape, Level Set-Discrete Element Method (LS-DEM)

1. Introduction

At the micro-scale considered by Discrete Element Methods (DEM), granular soils reveal diverse grain's shapes, that constitute one ingredient of their discrete nature. This shape enters soil classification and is directly used in geotechnical

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5 engineering for the ballast foundations of railtracks, which rely over angular,
6 not spherical, particles. Outside of this practical example, particle shape has
7 been recognised as influencing the mechanical behavior of granular materials
8 since several studies often adopting DEM approaches. In an early 2D study
9 on rotating cylinders and heap configurations (Pöschel and Buchholtz, 1993), a
10 non-spherical shape was shown to contribute even more to macro-behavior than
11 contact friction in the sense non spherical particles in frictionless interaction re-
12 vealed a higher slope stability than spherical particles in frictional interaction.
13 For a given frictional interaction, a higher shear strength of non-spherical par-
14 ticles has also been found for biaxial configurations in other 2D studies (Szarf
15 et al., 2009; Jerves et al., 2016), together with a shape influence onto the critical
16 state line (Jerves et al., 2016).

17 Investigating the mechanical influence of shape in real 3D conditions re-
18 mains however technically challenging. While experimental studies require a
19 proper particle-scale characterization of the complex shapes exhibited in nature
20 (Vlahinić et al., 2014; Wang et al., 2019), those same real shapes have to be
21 correctly introduced in the numerical world for DEM approaches. This induces
22 a much more complex contact treatment in the DEM workflow, as opposed to
23 the use of spherical particles which entails straightforward definitions of con-
24 tact normals and relative displacements from the branch vector and the radii of
25 contacting spheres. These complex contact treatments may obey several strate-
26 gies which are partially listed in the following. First, rigid clusters of spheres
27 (Pöschel and Buchholtz, 1993; Szarf et al., 2009; Garcia et al., 2009) enable the
28 DEM practitioner to get much closer to real shapes, making these rigid clusters
29 probably the second most-commonly used shape for Discrete Elements, just
30 after spheres. These clusters nevertheless inherently include some unrealistic
31 local roundness that may affect the mechanical description (Cho et al., 2006).
32 Convex polyhedra (Eliáš, 2014; Gladkyy and Kuna, 2017) now constitute another
33 quite classical shape enhancement since Cundall (1988), thanks to a variety of
34 algorithms such as searching for surface points with a common normal and/or
35 minimizing interparticle distance (Dubois, 2011). As described by Zhao and

36 Zhao (2019), some of those algorithms can also be adapted to superellipsoids
37 and quite general convex shapes without any edges. A last DEM variant to be
38 mentioned is the Level Set-DEM (LS-DEM) proposed in 3D by Kawamoto et al.
39 (2016). LS-DEM appears as promising in terms of versatility, since it does not
40 include any inherent requirement for convexity and may apply directly to X-ray
41 tomography images of soil samples (Kawamoto et al., 2016). Level Set concepts
42 were initially proposed to study time evolutions of surfaces (Sethian, 1999), and
43 applied in this sense to geotechnics by Golay et al. (2010, 2011) for flow-induced
44 interfacial soil erosion. In the sense of LS-DEM, those Level Set concepts are
45 used for defining in space distance fields to particles' surfaces, that are at the
46 heart of contact treatment.

47 One can finally think about introducing more complex contact laws as an in-
48 direct description of particle's shape (Wensrich and Katterfeld, 2012; Aboul Hosn
49 et al., 2017). However, this strategy obviously induces additional model param-
50 eters and increased calibration efforts that diminish the appealing mechanical
51 simplicity of DEM.

52 Advocating therefore for a direct description of particle's shape through e.g.
53 LS-DEM, the present manuscript then aims to discuss associated technical as-
54 pects in terms of obtained precision and increased computational costs, in the
55 case of an implementation based on the YADE code (Šmilauer et al., 2015). De-
56 tailed information in these technical aspects seem lacking until now, even though
57 one can await significant costs from the mentions of gigabytes RAM footprint in
58 (Kawamoto et al., 2016) or superprocessors with 480 cores in (Kawamoto et al.,
59 2018).

60 Section 2 presents the YADE implementation of LS-DEM based on the prin-
61 ciples given by Jerves et al. (2016); Kawamoto et al. (2016). Section 3 discusses
62 the variable precision of LS-DEM in describing contact- or packing-scale config-
63 urations adopting spherical or superellipsoid shapes: ideal spherical shapes are
64 in particular considered for the precision analysis to ground on reference results
65 obtained using DEM. LS-DEM precision is then connected with computational
66 costs in Section 4, before that parallel scalability is examined in Section 5 in

67 order to alleviate time costs.

68 2. Outline of LS-DEM

69 2.1. Shape description

70 Describing shape, i.e. particle morphology, in LS-DEM relies on the signed
 71 distance function $\phi(\vec{x})$ that returns, for any point \vec{x} in space, the shortest dis-
 72 tance from \vec{x} to the surface at hand, with the convention of negative distances
 73 when \vec{x} lies inside the surface. The surface of a Discrete Element (DE) then
 74 corresponds to the zero level set of the function ϕ , while the exterior (resp.
 75 inner) to the surface obeys $\phi > 0$ (resp. $\phi < 0$).

76 In this sense, LS-DEM is similar to the potential particles approach proposed
 77 by Houlsby (2009); Boon et al. (2013) where the sign of a potential function f
 78 defines the position of any point with respect to particle's surface, with $f =$
 79 0 along the surface. Potential particles however require convex shapes and
 80 polynomial equations for the potential f , unlike LS-DEM.

81 In LS-DEM, the signed distance function ϕ is actually defined in a dis-
 82 crete fashion, storing ϕ -values on a cartesian body-centered grid, for each DE
 83 (Figure 1). This minor requirement of a discrete distance field, instead of an
 84 analytical equation, confers LS-DEM a great versatility to mimic real shapes,
 85 as exemplified by Kawamoto et al. (2016, 2018).

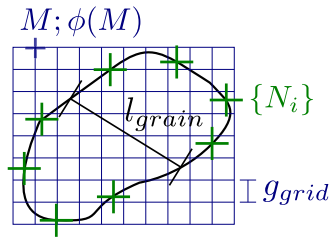


Figure 1: Plane view of the 3D regular grid at the roots of shape description in LS-DEM. Exact values of the signed distance function ϕ are known at each grid node M (the blue cross evidences just one of them). Boundary nodes N_i play a role in contact treatment as described in §2.2

86 From the knowledge of ϕ -values at each node of the grid, $\phi(\vec{x})$ is also defined
 87 for any point \vec{x} within the grid extents from trilinear interpolation of ϕ -values

88 at the eight surrounding grid nodes. In addition to defining particle’s surface,
 89 and serving for contact treatment as described in the following section 2.2, this
 90 distance field also enables one to define inertial quantities for DE summing mass
 91 and inertia contributions of all grid voxels that are considered inside a particle.
 92 Here, a grid voxel made of eight nodes $\{(i, j, k) ; i \in [i_0; i_0 + 1], j \in [j_0; j_0 + 1], k \in$
 93 $[k_0; k_0 + 1]\}$ is considered inside a particle depending on ϕ -value at the lowest
 94 node (i_0, j_0, k_0) . A smoother description was proposed by Kawamoto et al.
 95 (2016) but is not considered here, having in mind quasi-static simulations with
 96 no influence from the inertial quantities onto the results.

97 As will be discussed in more detail in section 3, the grid spacing g_{grid} , com-
 98 pared with particle’s characteristic length l_{grain} obviously affects the precision
 99 of the interpolated distance field, and that of LS-DEM.

100 Moreover such a distance field, the contact algorithm precised below in § 2.2
 101 introduces a second key ingredient for the method, since a LS-DEM shape also
 102 involves a set of so-called boundary nodes, being exactly located on the surface
 103 (Figure 1). These are obtained through ray tracing (e.g. Lin and Ching, 1996):
 104 starting from the center of mass of a DE, as determined from the inside voxels,
 105 a half-line ray defined by its direction \vec{v} is followed until crossing the DE’s
 106 surface. Rays \vec{v} could be chosen adopting various partitions of the (θ, φ) space,
 107 with $\theta \in [0; \pi]$ and $\varphi \in [0; 2\pi]$ being the two spherical angles. Here, boundary
 108 nodes follow a spiral path in the spirit of (Rakhmanov et al., 1994), where a
 109 total number N_{nod} of boundary nodes is located along the following spherical
 110 coordinates (θ_k, φ_k) , $k \in [0; N_{nod} - 1]$:

$$\theta_k = \arccos\left(-1 + \frac{1 + 2k}{N_{nod}}\right) \quad (1)$$

$$\varphi_k = \pi(3 - \sqrt{5})k \quad (2)$$

111 For spheres at least, such a spiral path seeds boundary nodes more uniformly
 112 over the particle’s surface, when compared with a rectangular partition of the
 113 (θ, φ) space. As a matter of fact, it avoids an overdiscretization of the poles
 114 ($\theta = 0 [\pi]$) thanks to the non-constant step in θ . For each ray direction \vec{v} , and

115 due to the trilinear description of distance within each grid voxel, the ray-surface
116 intersection can be obtained solving the roots of a cubic polynom, giving the
117 position of boundary nodes.

118 As it will be detailed in the following paragraph, no real update of the
119 boundary nodes, nor of the distance field is needed during LS-DEM simulations:
120 considering rigid particles with constant shapes, both are determined once for
121 all at the beginning of a simulation, in reference configurations of the DE.

122 The present shape description appears as very general and distance fields
123 for non-convex shapes could be readily obtained through Level Set algorithms
124 (Sethian, 1999) that also apply to such cases. Ray traced boundary nodes may
125 also follow non-convex shapes, with the only limitation being that ray tracing
126 leads to a maximum of one boundary node per grid cell, along a given ray, due
127 to the trilinear description of the distance field.

128 *2.2. Kinematics of contact from Level Set shape and boundary nodes*

129 Contact detection between two Level Set-shaped DEs first implies an ap-
130 proximate neighbour search that is common to all YADE simulations, following
131 a so-called sweep and prune algorithm working on bodies' axis-aligned bound-
132 ing boxes (Dubois, 2011; Šmilauer et al., 2015). This leads to a reduced list of
133 potential contacts between bodies pairs.

134 Exact determination of contact between two bodies in this list then relies
135 on a master-slave algorithm whereby the exact determination of interparticle
136 distance both relies on the distance field ϕ_B to the biggest (in volume) particle,
137 and on the boundary nodes \overrightarrow{ON}_i (with O the origin) of the smallest particle
138 (Figure 2). For convenience, labels 1,2 will replace in the following the mention
139 of small or big particles, with $\phi_2 = \phi_B$. Contact is then obtained for at least
140 one boundary node \overrightarrow{ON}_i showing $\phi_2(\overrightarrow{ON}_i) \leq 0$. Boundary nodes logically need
141 to be numerous enough to avoid bias in the LS-DEM results through missing
142 contacts if $\phi_2(\overrightarrow{ON}_i) > 0 \forall N_i$, as it will be investigated in the following sections.

143 After detecting at least one boundary node of 1 touching 2, the interaction
144 description is based on the node N_c showing the greatest penetration, leading

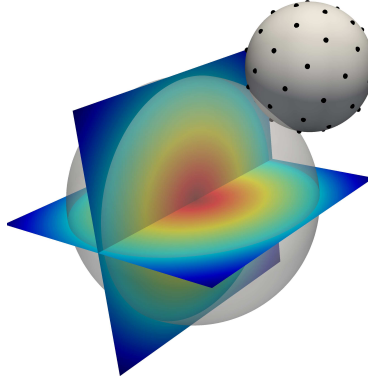


Figure 2: Distance field (colored map) and boundary nodes (black points) serving for the LS-DEM contact algorithm, illustrated for spherical particles

145 to the following interparticle overlap u_n :

$$u_n = -\min(\phi_2(\overline{ON}_i), \overline{ON}_i \in \mathcal{S}_1) = -\phi_2(\overline{ON}_c) \geq 0 \quad (3)$$

146 The current “greatest penetration” choice follows classical contact laws in DEM
 147 and corresponds to another recent LS-DEM study (Li et al., 2019). On the other
 148 hand, LS-DEM was initially proposed by Jerves et al. (2016); Kawamoto et al.
 149 (2016) with a mechanical interaction at each contacting node, which used to
 150 make the model behavior directly dependent on the number of boundary nodes,
 151 in addition to the k_n and k_t stiffnesses discussed below. That other choice would
 152 still enable to address non-convex shapes, which is not done here.

153 While the overlap u_n serves as the normal relative displacement, the present
 154 contact treatment does not resort to any total tangential displacement but just
 155 to an incremental one at the subsequent stage of applying the contact law, see
 156 the next § 2.3. The normal and tangential contact directions actually refer to
 157 the normal to \mathcal{S}_1 at N_c , chosen as the contact normal:

$$\vec{n} = \vec{\nabla} \phi_1(\overline{ON}_c) \quad (4)$$

158 For simplicity, special shapes showing pathological definitions of the normal,
 159 with tips or edges, are not considered here.

160 For e.g. the purpose of subsequent torque computations, a contact point \vec{x}_c

161 is defined in the middle of the overlap between 1 and 2:

$$\vec{x}_c = \overrightarrow{ON_c} - \frac{u_n}{2} \vec{n} \quad (5)$$

162 Considering the rigid bodies transformations of 1 and 2, the current contact
 163 algorithm easily makes use of the initial distance field and boundary nodes, as
 164 defined in the previous § 2.1 in reference configurations.

165 In line with its master-slave nature, such a contact treatment is not sym-
 166 metric and this could be seen as a possible source of inaccuracy in the contact
 167 model in the sense different results could have been obtained adopting other
 168 choices, using e.g. ϕ_2 instead of ϕ_1 in Eq. (4). It is however reasonably believed
 169 that a sufficient discretization of particle's surfaces with many boundary nodes
 170 would cancel this possible bias. One should also note that the present choice of
 171 the smallest particle for carrying the boundary nodes allows to explore distance
 172 fields (whose precision depends upon grid resolution only) with the greatest
 173 surface density in nodes.

174 2.3. Mechanics of contact

175 Once a contact is detected and kinematically described as presented in the
 176 above, classical elastic (resp. elastic-plastic) contact laws apply in the normal
 177 (resp. tangential) directions, with k_n and k_t the normal and tangential stiffnesses
 178 and μ the contact friction coefficient.

179 The repulsive normal force \vec{F}_n is first given by:

$$\vec{F}_n = k_n u_n \vec{n} \quad (6)$$

180 In the tangent plane, the frictional tangential force is incrementally com-
 181 puted from $\vec{0}$, one time step after another as per the following equation:

$$d\vec{F}_t = d \left(\|\vec{F}_t\| \frac{\vec{F}_t}{\|\vec{F}_t\|} \right) = \|\vec{F}_t\| d \left(\frac{\vec{F}_t}{\|\vec{F}_t\|} \right) + d(\|\vec{F}_t\|) \frac{\vec{F}_t}{\|\vec{F}_t\|} \quad (7)$$

182 In the rhs of Eq. (7), the first term just accounts for a possible change in
 183 the tangential force direction (its unit vector $\vec{F}_t/\|\vec{F}_t\|$) while the interacting
 184 pair would move as a rigid body with possible variations in the orientation of

185 the tangent plane. This first term is computed from the previous and current
 186 normal directions and from the angular velocities of each DE (Šmilauer et al.,
 187 2015). On the contrary, the last term in Eq. (7) accounts for the force variation
 188 due to a incremental tangential relative displacement, $d\vec{u}_t$, as computed at the
 189 contact point between the two DEs. A classical elastic-plastic force-displacement
 190 relationship here applies:

$$d(\|\vec{F}_t\|) \frac{\vec{F}_t}{\|\vec{F}_t\|} = k_t d\vec{u}_t \quad \text{enforcing } \|\vec{F}_t\| \leq \mu \|\vec{F}_n\| \quad (8)$$

191 The interaction force being determined, an associated torque is also imposed
 192 with a possible contribution of the normal force for arbitrary shapes, unlike
 193 spheres.

194 *2.4. Equations of motion*

195 Sustaining resultant forces and torques, each DE is classically characterized
 196 in space using $\vec{x}(t)$, the current position of its center of mass P , as well as a
 197 rotation matrix $\mathbf{R}(t)$ that describes its current orientation, i.e. the orientation
 198 of the local frame of eigenvectors for the inertia matrix, $(\vec{e}_i), i \in [1; 3]$, as seen
 199 in the global frame. The rotation matrix \mathbf{R} actually transforms each vector \vec{u}_L
 200 of the local frame in its current counterpart in the global frame \vec{u}_G through
 201 classical change of basis relation $\vec{u}_G = \mathbf{R}\vec{u}_L$. Newton-Euler equations for the
 202 motion of rigid bodies then rule the evolutions of \vec{v} , the velocity of point P and
 203 of $\vec{\omega}$, the angular velocity of the body:

$$m \frac{d\vec{v}}{dt} = \vec{f} \quad (9)$$

$$\mathbf{I} \frac{d\vec{\omega}}{dt} + \vec{\omega} \wedge \mathbf{I} \vec{\omega} = \vec{\Gamma} \quad (10)$$

204 , with \vec{f} the resultant force on the DE and $\vec{\Gamma}$ the resultant torque computed
 205 at the center of mass P . For the purposes of deriving Eq. (10) $\vec{\Gamma}$ and $\vec{\omega}$ are
 206 expressed in the local frame (\vec{e}_i) , where \mathbf{I} components are constant. We recall
 207 that Eq. (10) would simplify to $\mathbf{I} d\vec{\omega}/dt = \vec{\Gamma}$ for simple, isotropic, shapes with a
 208 spherical inertia matrix $\mathbf{I} = k\delta$ (with δ the identity matrix), such as spheres or
 209 cubes.

210 Global damping is classically considered, modifying the resultant forces and
 211 torques in Eqs. (9)-(10) in dynamic cases where those are non-zero. A damping
 212 coefficient D , taken here equal to 0.2, enters the equations such that the right
 213 hand sides of Eqs. (9)-(10) actually are $(1 \pm D)\vec{f}$ or $(1 \pm D)\vec{\Gamma}$, depending on the
 214 power of resultant forces or torques. Accelerating cases with a positive power
 215 are hindered, considering $(1 - D)$, while decelerating conditions with a negative
 216 power are amplified through the use of $(1 + D)$.

217 Time variations of position and orientation finally follow from the above
 218 Newton-Euler equations as per:

$$\frac{d\vec{x}}{dt} = \vec{v} \quad (11)$$

$$\frac{d\mathbf{R}}{dt} = \mathbf{R}\mathbf{\Omega} \quad (12)$$

219 , with $\mathbf{\Omega}$ in Eq. (12) being the antisymmetric matrix such that $\mathbf{\Omega}\vec{x} = \vec{\omega} \wedge \vec{x}$,
 220 $\forall \vec{x}$. Integrating these Eqs. (9) to (12) is achieved in YADE from appropriate
 221 explicit numerical schemes and using a quaternion equivalent for the rotation
 222 matrix \mathbf{R} (Šmilauer et al., 2015).

223 3. Precision of LS-DEM

224 3.1. Materials and methods

225 The precision of LS-DEM in connection with boundary nodes and grid spac-
 226 ing is now investigated for different kinds of numerical simulation, comparing
 227 when possible LS-DEM with classical DEM serving as a numerical reference.
 228 For comparison purposes, ideal spherical shapes are then often adopted, since
 229 they enable one to obtain such a DEM reference result. The distance fields
 230 necessary to LS-DEM are straightforward to define for spheres of given radii.

231 Extending towards arbitrary shapes, superellipsoids, also known as super-
 232 quadrics (Barr, 1995), are also considered. Generalizing ellipsoids, they consti-
 233 tute a convenient choice for exploring non-spherical shapes, e.g. (Wang et al.,
 234 2019), since they offer an analytical description through three radii r_x, r_y, r_z
 235 distorting length along the three axes, combined with two additional exponents

Shape index	Half-extents (length unit)			Curvature exponents (-)	
	r_x	r_y	r_z	ϵ_e	ϵ_n
0	0.4	1	0.8	0.4	1.6
1	0.42	=	0.83	0.1	1
2	=	=	=	1	0.5
3	0.5	0.7	1	1.4	1.2

Table 1: Shape parameters of the four superellipsoids shown in Figure 3

236 ϵ_e , ϵ_n that modify the surface curvature. In local axes, their surface equation
237 namely reads:

$$f(x, y, z) = \left(\left| \frac{x}{r_x} \right|^{\frac{2}{\epsilon_e}} + \left| \frac{y}{r_y} \right|^{\frac{2}{\epsilon_e}} \right)^{\frac{\epsilon_e}{\epsilon_n}} + \left| \frac{z}{r_z} \right|^{\frac{2}{\epsilon_n}} - 1 = 0 \quad (13)$$

238 While such an analytical description is not required in LS-DEM, it aptly provides
239 a first order approximation for the signed distance function to a superellipsoid,
240 which is herein simply proposed as:

$$\phi \approx \frac{f}{\|\vec{\nabla} f\|} \quad (14)$$

241 Eq. (14) obviously describes a zero distance, $\phi = 0$, along the surface. It is
242 furthermore easily verified that the Eikonal equation defining distances, $\|\vec{\nabla} \phi\| =$
243 1 (Sethian, 1999), is by construction verified at the first order close to the
244 surface. This approximation, illustrated in Figure 3, is sufficient for typical
245 LS-DEM simulations with negligible overlaps since an accurate distance field is
246 then necessary close to the surface only.

247 The Table 1 lists a chosen set of 4 shape parameters, with the corresponding
248 4 different superellipsoids being depicted in Figure 3. The radii r_x , r_y , r_z shown
249 therein will be scaled to appropriate lengths in the following.

250 Regardless of the shape or the modelling approach (DEM or LS-DEM) cho-
251 sen thereafter, the same contact parameters and particle size distribution are
252 used, see Table 2. The distribution of particle's diameter D is uniform in number
253 between extreme D_{min} and D_{max} , whose values do not necessarily correspond to
254 any physical entity. Numerical samples made of superellipsoids include in equal
255 proportion the 4 shapes presented in the above and conform that same particle

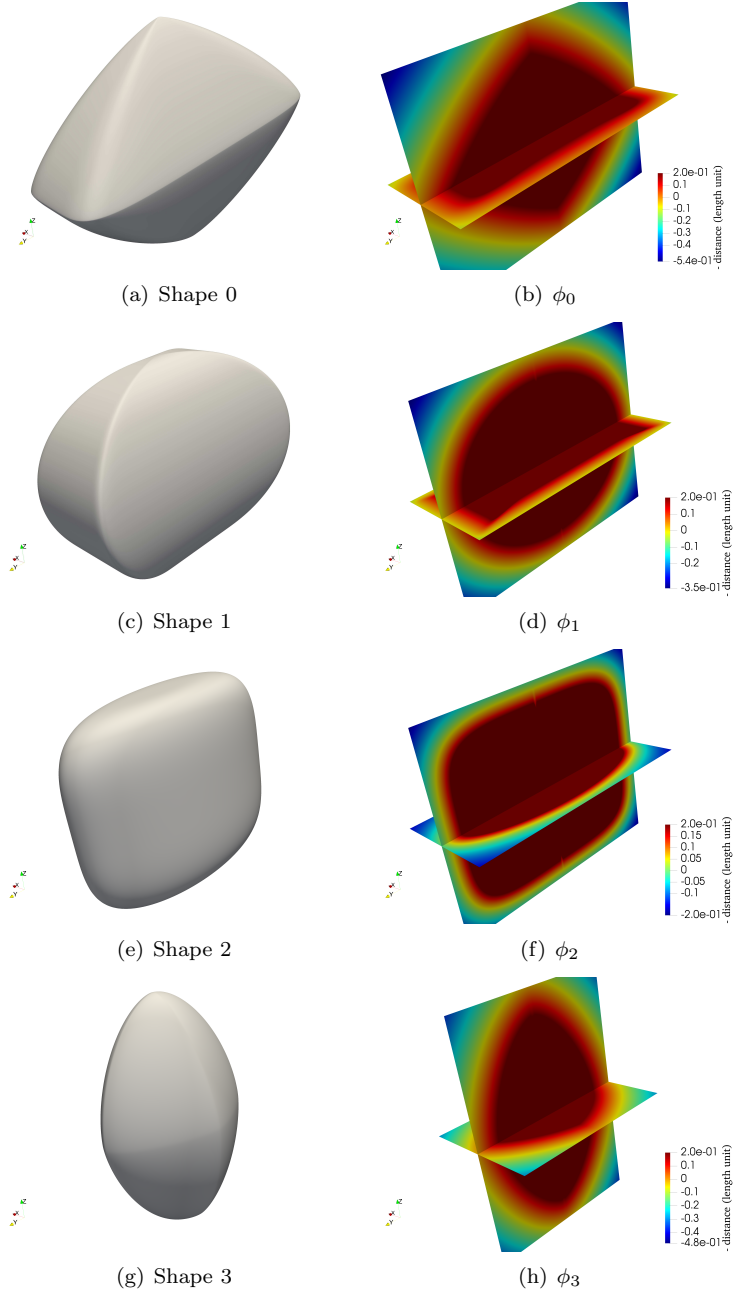


Figure 3: The four superellipsoids (left) defined in Table 1, illustrated together with their distance fields (right). Image scales are constant for each shape (on each row), and the positive range of color maps (shape's interior) is capped to 0.2 length units for convenience

256 size distribution. Doing so, a sieve diameter is chosen for each superellipsoid as
 257 the diameter of its circumscribed sphere, i.e. twice the greatest center-boundary
 258 node distance.

Table 2: DEM and LS-DEM mechanical parameters

k_n (N/m)	k_t/k_n (-)	μ (-)	D_{min} (cm)	D_{max}/D_{min} (-)
6×10^5	0.3	0.577	6.1	3

259 3.2. Single contact description

260 The precision of LS-DEM is first analyzed for the simple case of a single
 261 contact between two spherical particles, with a possible discrepancy in size (Fig-
 262 ure 2). While the precision of each particle’s distance field is fully defined by
 263 the resolution D/g_{grid} of its underlying grid, the ability of the LS-DEM contact
 264 algorithm to capture the distance field furthermore depends upon boundary
 265 nodes, in the number of N_{nod} , and on the diameter ratio $D_2/D_1 \geq 1$. The
 266 Figure 4 illustrates how these three parameters affect the LS-DEM measure of
 267 an overlap between the two spherical particles.

268 It is for instance observed in Figure 4(a) that using just 100 boundary nodes
 269 (in 3D space) leads to miss interactions close to the unit circle of the map, and
 270 to an approximation between the detected overlap and the true distance to a
 271 sphere. On the other hand, the Figure 4(d) confirms the true distance field can
 272 be re-obtained with a very good precision, i.e. $u_n = -\phi$, using $D/g_{grid} = 50$
 273 and $N_{nod} = 1600$, with $D_2/D_1 = 1$. Thanks to the present choice of locating
 274 boundary nodes on the smallest sphere, cases with $D_2/D_1 > 1$ are described
 275 with a greater precision, see Figure 4(b) vs 4(a).

276 3.3. Isotropic reconstruction

277 A second examples devotes to the LS-DEM reconstruction of a dense pack-
 278 ing of 8000 spherical particles. While the current reconstruction procedure is
 279 essentially similar to the definition a LS-DEM sample from an experimental
 280 one, e.g. through computed tomography (Kawamoto et al., 2016, 2018), it ac-
 281 tually here applies to DEM data describing the isotropic state of a numerical

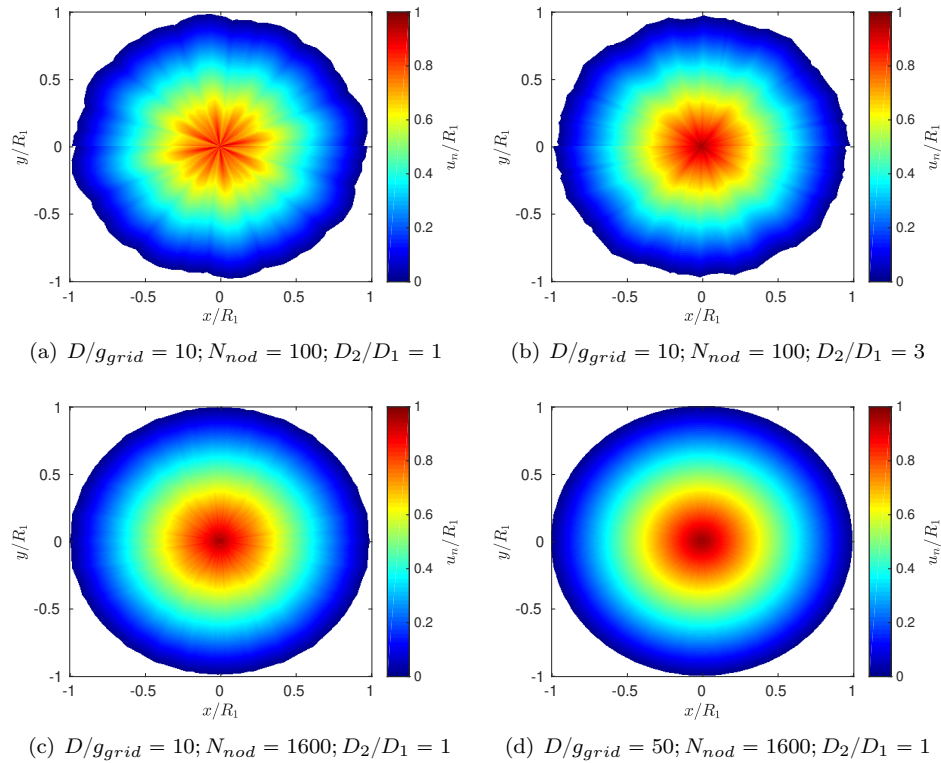


Figure 4: Precision of the LS-DEM contact algorithm in capturing a sphere's distance field. Color maps show the overlap $u_n(x, y)$ of a LS-DEM interaction between a sphere 1 centered at (x_c, y_c, z_c) and a bigger sphere 2 centered at $(x_c + (r + R_2) \cos(\theta), y_c + (r + R_2) \sin(\theta), z_c)$ with (r, θ) the polar counterparts to the cartesian (x, y) . The origin of the map, $x = y = 0$, for instance corresponds to the center of 1 belonging the surface of 2, and to an expected overlap value equal to R_1 . White region correspond to the absence of an interaction. Each map is constructed using 401^2 colored pixels and as many relative configurations of the two spheres

282 sample, showing a $n_{ref} \approx 0.372$ porosity while subjected to an hydrostatic
 283 pressure $p_{ref} = 16.5$ kPa. This pressure value corresponds to a stiffness ratio
 284 $\kappa = k_n/(pD_{50}) \approx 300$ which is an intermediate value among DEM studies. One
 285 can for instance mention κ -values in the order of several hundreds up to one
 286 thousand in qualitative (Duriez et al., 2018) as well as quantitative (Aboul Hosn
 287 et al., 2017) studies.

288 As such, a first DEM simulation, whose parameters were presented in Ta-
 289 ble 2, is run to reach that mechanical state. After exporting from the DEM
 290 model the positions and diameters D of all spherical particles, a LS-DEM recon-
 291 struction is attempted using at the particle scale different numbers of boundary
 292 nodes $N_{nod} \in \{0;100;400;900;1200;1600;2000;2500;4000;9000\}$ and grid resolu-
 293 tion $D/g_{grid} \in \{10;20;30;50;90\}$. LS-DEM spheres being so defined from known
 294 positions and radii, reconstructed porosity n can be measured and one LS-DEM
 295 iteration is finally performed in order to also reconstruct normal contact forces
 296 being responsible for the sample’s mean stress p , while preventing any move-
 297 ments of the DE. The obtained precision in terms of porosity or mean stress can
 298 be quantified through the n/n_{ref} or p/p_{ref} ratios, where a value of 1 or 100%
 299 indicates a perfect LS-DEM reconstruction of the reference case.

300 Porosity precision is actually independent of the boundary nodes and can
 301 be seen as geometric in nature since voxellised particles volumes are fully de-
 302 termined from the grid resolution. As such, the Figure 5 disregards boundary
 303 nodes number N_{nod} and evidences how spherical morphologies can be satisfac-
 304 torily described with tens of grid voxels per diameter, with the error on porosity
 305 i.e. solid volumes reducing below 4% for $D/g_{grid} \geq 20$.

306 On the other hand, in terms of mean stress p/p_{ref} data (Figure 6) illustrate
 307 how grid resolution and boundary nodes both contribute to the mechanical
 308 precision of LS-DEM. Starting from an absence of contacts and stress in the ex-
 309 treme case of $N_{nod} = 0$, boundary nodes obviously have to be numerous enough
 310 for all contacts to be detected. For a given number of boundary nodes, grid
 311 resolution still improves precision since it contributes to more exact locations of
 312 these boundary nodes, closer to the true surface, as well as to a better overlap

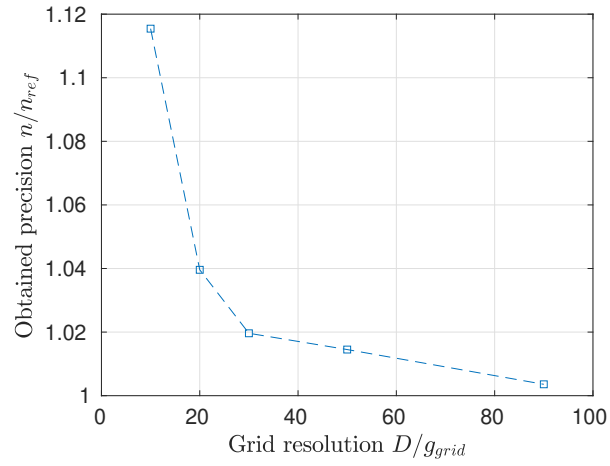


Figure 5: Geometric precision of LS-DEM in terms of porosity n after reconstructing a fully determined spherical packing in isotropic state

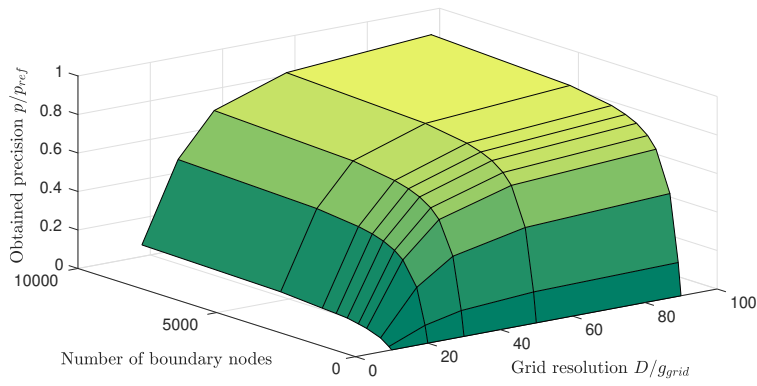


Figure 6: Mechanical precision of LS-DEM in terms of mean stress p after reconstructing a fully determined spherical packing in isotropic state. Each vertex of the depicted surface corresponds to one LS-DEM reconstruction

313 estimation. As a matter of fact, a 80% precision can here be obtained choos-
 314 ing $\{N_{nod}; D/g_{grid}\}$ either as $\{2500;50\}$ or $\{1600;90\}$. Among the cases tested,
 315 a maximum precision of 94 % is reached for 9000 boundary nodes and a grid
 316 resolution of 90, which is another step towards validating the present LS-DEM
 317 implementation with respect to DEM and investigating the role of its technical
 318 ingredients $\{N_{nod}; D/g_{grid}\}$. This is pushed further in the following section.

319 *3.4. Triaxial compression*

320 Another comparison between DEM and LS-DEM for spherical shapes even-
 321 tually considers the triaxial compression of that same dense sample, under the
 322 confining stress $\sigma_2 = \sigma_3 = 16.5$ kPa and until an axial strain $\varepsilon_1 = 5$ %. This
 323 axial strain value is posterior to the peak in deviatoric stress $q = \sigma_1 - \sigma_3$ that
 324 is observed in DEM.

325 Again, several LS-DEM simulations are carried on, for $N_{nod} \in \{100;400;1600;$
 326 $2500;4000\}$ and $D/g_{grid} \in \{10;20;50\}$. Any LS-DEM simulation starts with the
 327 same sample definition than before, defining appropriate Level Set shaped bod-
 328 ies from the DEM data that describe the isotropic stress $p_{ref} = 16.5$ kPa.
 329 Because the same mechanical state is not directly captured within LS-DEM,
 330 confining phase is pursued further, with a servo-control of boundary walls un-
 331 til that reference isotropic stress p_{ref} is re-obtained. Then, both DEM and
 332 LS-DEM simulations apply triaxial shear loading with a constant axial strain
 333 rate $\dot{\varepsilon}_1$ that corresponds to an inertial number $I = \dot{\varepsilon}_1 D_{50} \sqrt{\rho/\sigma_3} \approx 10^{-4}$ low
 334 enough for its influence and the one of global damping to vanish. It is actually
 335 verified in DEM and LS-DEM that stresses measured along the boundary walls
 336 equal homogenized Love-Weber stresses (Love, 1892; Weber, 1966; Drescher and
 337 de Josselin de Jong, 1972) for static equilibrium conditions. Table 3 details rele-
 338 vant parameters, with a fictitious $\rho = 1000$ kg/m³ density being herein adopted.
 339 The latter could be replaced by another value provided that time step and load-
 340 ing rate are also modified in order to avoid divergence of the explicit scheme and
 341 maintain the same inertial number. Such changes would keep constant the total
 342 number of DEM iterations required for simulating triaxial shear until $\varepsilon_1 = 5$ %.

Table 3: DEM and LS-DEM numerical parameters for the triaxial compressions

Density ρ (kg/m ³)	Timestep		Damping coefficient D (-)	Loading rate $\dot{\epsilon}_1$ (s ⁻¹)
	Δt (s)			
	Spheres	Superquadrics		
1000	3.4×10^{-4}	1.7×10^{-4}	0.2	2.5×10^{-3}

343 On that second example, the LS-DEM precision is quantified comparing the
 344 deviator peak q^{max} of each LS-DEM simulation with the reference DEM value
 345 $q_{ref}^{max} \approx 33$ kPa, through a q^{max}/q_{ref}^{max} ratio that is illustrated in the Figure 7.

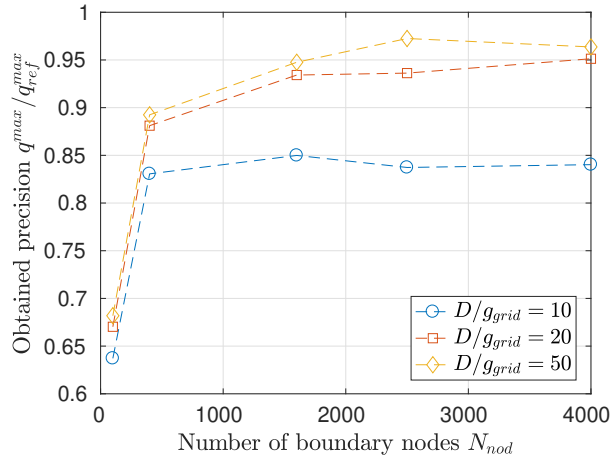


Figure 7: Precision of LS-DEM in terms of peak strength during the triaxial loading of spherical grains

346 Similar trends in precision are observed on this third example, with a joint
 347 influence of the grid resolution and the number of boundary nodes. This be-
 348 ing said, the present DEM *vs* LS-DEM comparison with non-fixed DEs un-
 349 der deviatoric loading is more favorable than the isotropic reconstruction. In-
 350 deed, using 4000 boundary nodes and a grid resolution of 50 now enables
 351 one to reach an excellent 96% overall precision, whereas it previously led to
 352 just 85% for the isotropic example. This 85% precision would here be ex-
 353 ceeded choosing $\{N_{nod} = 400; D/g_{grid} = 20\}$ only. The particular case of
 354 $\{N_{nod} \geq 1600; D/g_{grid} = 10\}$ illustrates the marginal possibility for a non-
 355 monotonous increase in precision with respect to N_{nod} . One may think for

instance to the very specific case of two spheres in contact that could be perfectly described with just one boundary node located along their branch vector.

In addition to the only consideration of peak deviatoric stress, the Figure 8 illustrates the effects of $\{N_{nod}; D/g_{grid}\}$ choices onto the evolutions of other average quantities according to axial strain. LS-DEM is therein also compared with DEM for what concerns the volumetric strain ε_V , the anisotropy a_c of the contact network, and the average contact number z_c . As for the contact anisotropy a_c , the latter is expressed as the difference between the axial and the lateral components of the fabric tensor \mathbf{F} whose expression is represented in the following Eq. (15).

$$\mathbf{F} = \frac{1}{N_c} \sum_c \vec{n} \otimes \vec{n} \quad (15)$$

For the purpose of computing \mathbf{F} in LS-DEM, it is recalled contact normals are computed in this case from the distance gradient as per the previous Eq. (4). The precision in evaluating this distance gradient again depends on grid resolution.

The Figure 8 confirms that the LS-DEM evaluation of any quantity of interest tends to its DEM counterpart for $\{N_{nod}; D/g_{grid}\}$ reaching the order of $\{4000;50\}$. It furthermore illustrates how the dense-like behavior traits, with softening and dilation, of the present numerical sample appear as diminished when using an insufficient LS-DEM discretization in terms of boundary nodes and grid resolution. One can lastly note that LS-DEM curves are generally speaking somewhat more noisy than DEM counterparts, due to the surface discretization in boundary nodes. Such a surface discretization, when poor in particular, may indeed enhance the discontinuous i.e. sudden changes in overlap and contact forces already present in DEM due to the time discretization, possibly affecting the curves at the macro-scale.

3.5. Triaxial compression of superellipsoids

A last example devotes to a packing of 8000 superquadrics, as defined in the above § 3.1, under the same triaxial loading than the one imposed on spherical particles. After reaching the isotropic state (Figure 9) $p = 16.5$ kPa and $n \approx 0.32$ through compressing an initial cloud of superellipsoids, in a similar manner than

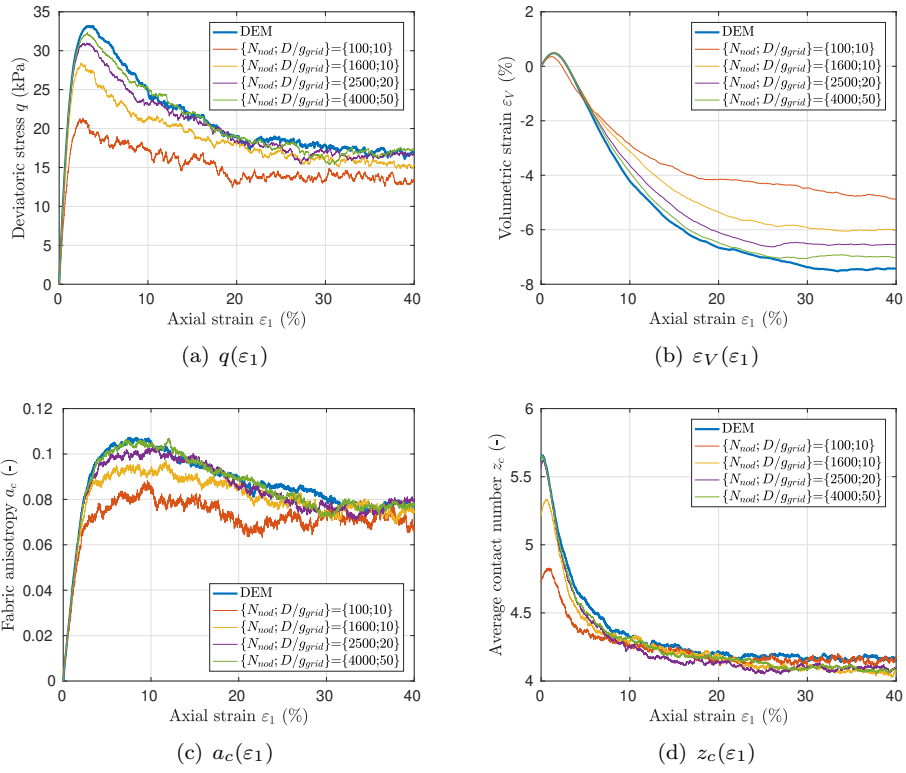


Figure 8: DEM vs LS-DEM comparisons during a triaxial loading of spherical grains: effects of LS-DEM discretization onto averaged quantities

385 for spheres, triaxial shear is again pursued until an axial strain $\varepsilon_1 = 5\%$ being
 386 posterior to the deviator's peak. Among the simulation parameters, being listed
 387 in Tables 2 and 3, time step is modified from the spherical case because of a
 388 possibly lower volume, hence mass, of a superellipsoid when compared to a
 389 sphere having the same circumscribed diameter.

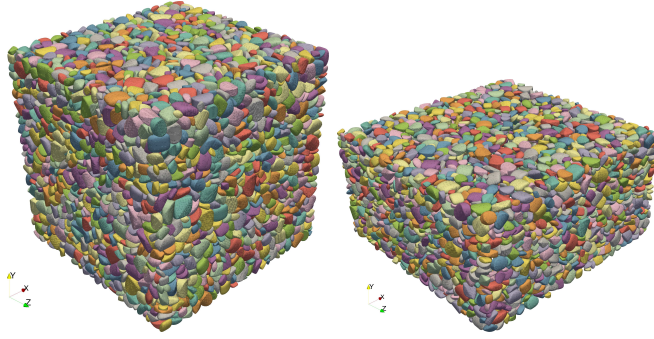


Figure 9: Initial (left) and sheared (right, for $\varepsilon_1 = 40\%$) configurations of the superellipsoids packing under triaxial loading

390 Such a LS-DEM simulation is carried on for different choices of $N_{nod} \in \{400;$
 391 $1600;2500;4000\}$ and $2 \min(r_x, r_y, r_z)/g_{grid} \in \{10;20;50\}$, disregarding here the
 392 less precise case $N_{nod} = 100$. Looking at the obtained peak in q , the data
 393 illustrated in the Figure 10 once again show how both the grid resolution and the
 394 boundary nodes number affect the LS-DEM results. With respect to the ideal
 395 spherical shapes considered in the above, the results also suggest that capturing
 396 more complex shapes might be more demanding in terms e.g. of boundary nodes
 397 number N_{nod} . While using $N_{nod} \geq 1600$ induced fairly constant LS-DEM results
 398 for spheres (within a 2-3% variation, see Figure 7), the present results on
 399 superellipsoids still vary by nearly 10% in that range, without a clear plateau.

400 As for the deviator strength itself, one can also note from the most pre-
 401 cise LS-DEM simulations that the superquadrics packing exhibits a deviator
 402 strength $q^{max} \approx 48$ kPa, which is approximately 45% higher than the ones for
 403 spheres (where $q_{ref}^{max} \approx 33$ kPa) and combined with differences in initial porosity
 404 or coordination number. A greater ultimate triaxial strength at critical state is
 405 also obtained, with $M = q/p \approx 0.76$ for spheres, versus $M \approx 1.13$ for superel-

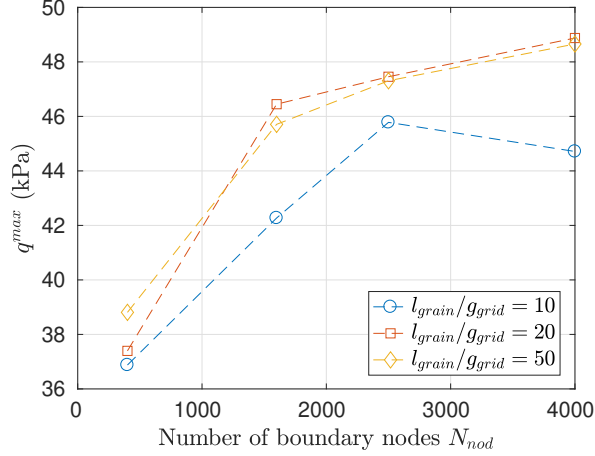


Figure 10: LS-DEM description of the peak strength for a triaxial loading imposed on superellipsoids, choosing $l_{grain} = 2 \min(r_x, r_y, r_z)$.

406 lipsoids using $N_{nod} = 2500$ and $2 \min(r_x, r_y, r_z)/g_{grid} = 20$ until $\varepsilon_1 = 40$ %.
 407 While further discussion is left for future work, these results confirm the shape
 408 influence upon the mechanical properties.

409 3.6. Discussion

410 From the comparisons shown in the above, and with a greater focus on the
 411 more meaningful triaxial simulation with moving DEs, one could advice to use a
 412 grid resolution (l_{grain}/g_{grid}) in the order of few tenths, and a couple of thousands
 413 boundary nodes at least. Even though previous LS-DEM studies (Jerves et al.,
 414 2016; Kawamoto et al., 2016, 2018) did not explicitly provide such technical
 415 details, similar order of magnitudes can be inferred as follows.

416 Regarding the boundary nodes, the key references (Jerves et al., 2016; Kawamoto
 417 et al., 2016) formulated the same guideline in terms of node-to-node spacing,
 418 proposing therein that restricting these distances to one tenth of particle diam-
 419 eter would avoid bias in the results. In addition to distance considerations, a
 420 proper set of boundary nodes should obviously cover the whole direction space
 421 $\theta \times \varphi = [0; \pi] \times [0; 2\pi]$. Assuming this was done in (Kawamoto et al., 2016) with
 422 a rectangular partition, and considering that $R\sqrt{\Delta\theta^2 + \Delta\varphi^2}$, with $\Delta\theta, \Delta\varphi$ the

423 increments in the spherical angles θ, φ between two adjacent nodes, is an upper
 424 bound to that node-to-node distance, one can connect node-to-node spacing to
 425 the increments $\Delta\theta, \Delta\varphi$, then to the total number of nodes N_{nod} . As such,
 426 the above distance guideline quoted by Jerves et al. (2016); Kawamoto et al.
 427 (2016) can eventually be related to a total number of nodes N_{nod} being in the
 428 order of 1200. The present comparisons rather confirm this order of magnitude
 429 of thousand of boundary nodes as a minimum, and they furthermore illustrate
 430 how the grid resolution articulates with N_{nod} for what concerns the precision of
 431 the method.

432 As for the grid resolution itself, no exact mention of the latter seems to be
 433 found in (Jerves et al., 2016; Kawamoto et al., 2016, 2018). One can nevertheless
 434 speculate from Kawamoto et al. (2016) that a resolution l_{grain}/g_{grid} in the order
 435 of 30 or 40 was adopted therein, which also appears to be the required order of
 436 magnitude.

437 To conclude, LS-DEM practice certainly requires to consider grid resolution
 438 and boundary nodes as similar technical ingredients than meshes for Finite
 439 Element Methods, and eventually to check their (non-)influence onto the results.

440 **4. Computational costs**

441 The greater flexibility of LS-DEM logically comes along greater computa-
 442 tional costs, be in terms of memory (RAM) footprint or evaluation time. These
 443 are now carefully investigated for the triaxial compression of spherical particles
 444 until $\varepsilon_1 = 5\%$ that was considered in the previous section 3.4, with the same
 445 choices of grid resolution D/g_{grid} and N_{nod} boundary nodes than before. The
 446 consideration of spheres allows once again direct comparisons with the classical
 447 DEM, but it is an interesting LS-DEM feature that computational costs are
 448 naturally insensible to the shapes being described, since they depend only upon
 449 grid resolution and boundary nodes number.

450 First of all, the RAM costs associated with the definition of DEs in LS-DEM
 451 are quantified and compared with the corresponding RAM cost in DEM. While
 452 the introduction of classical spheres here requires 10 megabytes of RAM for

453 a DEM simulation, LS-DEM requires 100 or 1000 times more, i.e. gigabytes
 454 (Figure 11(a)). An important RAM consumption obviously arises due to the
 455 distance grid and its distance values counting in the order of r^3 for a grid
 456 resolution $r = D/g_{grid}$, per particle. Boundary nodes also contribute to RAM
 457 footprint since $3 N_{nod}$ coordinate values have to be stored for each particle with
 458 N_{nod} boundary nodes. Several cases considered in previous sections 3.3 and 3.4
 459 make these two quantities comparable. The Figure 11(a) illustrates how RAM
 460 footprint is affected by boundary nodes number (then precision) for low grid
 461 resolution: $D/g_{grid} = 10$ or 20 , while being fairly constant for the finest grid with
 462 $D/g_{grid} = 50$. For such a fine grid, most storage requirements indeed concern
 463 the distance values, with, in proportion, little extra-requirements coming from
 464 the boundary nodes.

465 Second, evaluation costs are measured as the average wall clock duration of
 466 one iteration during the triaxial shearing. All LS-DEM simulations as well as
 467 the reference DEM simulations run sequentially as one thread executed on the
 468 same server machine. The server includes two Intel Xeon Platinum 8270, 2.7
 469 GHz, processors with 26 cores and 36 MB of cache memory each. It thus offers
 470 a total of 52 cores and 104 threads, together with 1.5 TB 2.9 GHz RAM. On
 471 that machine, LS-DEM execution takes approximately 25 to 300 times longer
 472 than classical DEM, depending on LS-DEM parameters such as N_{nod} . From a
 473 quantitative point of view, these observations should be cautiously interpreted
 474 since they suffer from a non-exactly reproducible nature of evaluation times, in
 475 connection e.g. with temperature changes. They furthermore certainly depend
 476 on the hardware and simulation at hand, and on the present implementation
 477 into the YADE code. The comparison nevertheless provides useful orders of
 478 magnitude for (LS-)DEM practitioners. From a qualitative point of view, the
 479 Figure 11(b) illustrates how the present time cost is primarily affected by the
 480 number of boundary nodes, with an increasing N_{nod} leading to longer loops for
 481 contact treatment, in the same time it globally improves precision. For a given
 482 N_{nod} , slight variations in time cost are observed depending on the grid resolu-
 483 tion D/g_{grid} , which just come from the previously mentioned non-reproducible

484 nature of evaluation times.

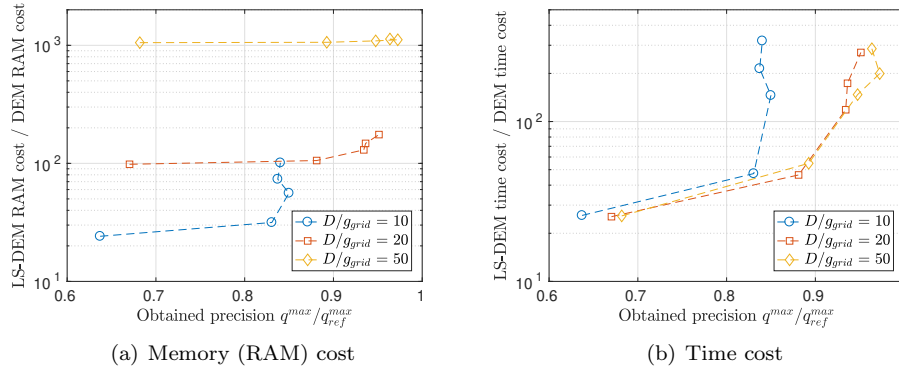


Figure 11: LS-DEM computational costs according to precision for the triaxial shear on spheres, relative to the costs of DEM. Each datapoint corresponds to the use of different numbers of boundary nodes N_{nod} , among $\{100;400;1600;2500;4000\}$, resulting into different costs and precision for a given grid resolution D/g_{grid}

485 Finally, the present cost analysis also recalls the combined influence of both
 486 boundary nodes and grid resolution onto the results. It actually illustrates the
 487 possibility for different strategies of ressource managements, when seeking a
 488 given precision. Aiming to limit RAM consumption, a 95% precision could be
 489 here obtained choosing $D/g_{grid} = 20$ and 4000 boundary nodes. On the other
 490 hand, choosing $D/g_{grid} = 50$ and 1600 boundary nodes would show higher mem-
 491 ory requirements, but would lead to the same precision after faster simulations.

492 5. OpenMP scalability for parallel simulations

493 Parallel computing is an obvious strategy to alleviate the high time costs of
 494 LS-DEM, and is available in YADE e.g. in a OpenMP shared memory frame-
 495 work (Šmilauer, 2010). The OpenMP framework distributes the treatment of
 496 DEM variables among parallel threads that will collectively move forward the
 497 simulation. Typical examples include integrating motion for different DEs with
 498 different threads, or the parallel computing of interaction forces for different
 499 interactions. However, the shared memory paradim inherently requires costly
 500 safeguards to avoid conflicts between possible operations from different threads

501 onto the same DEM variable. One can think for instance to the resultant force
502 of one given DE contributing to different interactions, which could be modi-
503 fied by different threads after parallel computations of interaction forces. After
504 performing extra-operations to avoid such pitfalls, OpenMP speedups in YADE
505 usually do not reach the optimal value of threads number (Šmilauer, 2010), with
506 possible peaks in speedup around 8 threads for spherical particles (Zhao and
507 Zhao, 2019).

508 As for LS-DEM, parallel speedups are investigated hereafter for the same
509 triaxial shear on spheres and until $\varepsilon_1 = 5\%$ than considered in the previous
510 sections 3.4 and 4, using 1600 boundary nodes and a grid resolution of 20 which
511 conferred LS-DEM a sufficient precision (93%). Allocating a variable number of
512 threads, the LS-DEM simulation is executed on the server machine mentioned
513 in the above section 4, as well as on a workstation with one 4 cores (8 threads)
514 Intel i7-7700, 3.60GHz processor with 8 MB of cache memory, as well as 64 GB
515 of 2.4 GHz RAM.

516 Allocated threads go from 1 to 8 for the workstation, and from 1 to 100 for
517 the server. For each thread number j (including the sequential case $j = 1$),
518 simulation time t is measured repeating 3 times the simulation to account for
519 the possible variations in time cost. Then, 9 parallel speedups can be measured
520 for a given j , through the 9 ratios $t(j)/t(j = 1)$.

521 After averaging among these 9 measurements and quantifying error as one
522 standard deviation, the data (Figure 12) show LS-DEM parallel simulations
523 follow a linear speedup until 22 threads approximately. Under those conditions
524 the workstation shows a fairly optimal speedup, while a 0.6 speedup coefficient,
525 40% smaller than the optimal one, is obtained on the server. Using even more
526 threads, simulations then continue to speed up, at a lower rate, until 50 threads
527 approximately. For that number of threads, parallel execution is more than 20
528 times faster than the sequential one. The simulation speed afterwards starts
529 to decrease with the number of threads, whereby allocating more resources
530 eventually just increases evaluation time.

531 Even though the OpenMP scalability is not necessarily optimal, significant

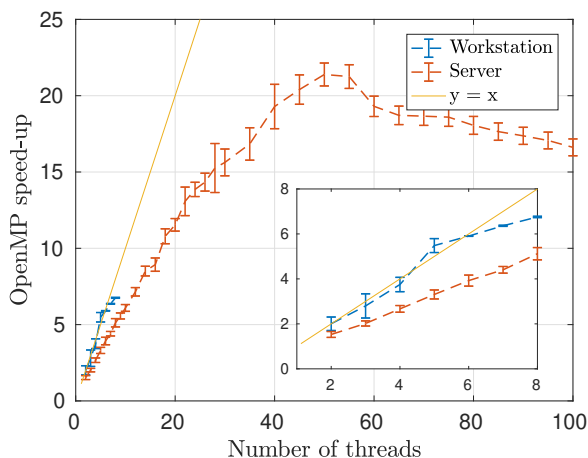


Figure 12: OpenMP speed up for the LS-DEM triaxial compression using spherical grains

532 time can then be saved in a LS-DEM simulation using an appropriate number
 533 of threads between 20 and 50. Time gains are even greater in proportion than
 534 one could get for classical DEM simulations. Indeed, the maximum parallel
 535 speed-up for the DEM simulation approximates 3.5 only, which is obtained for
 536 10 threads approximately (Figure 13). Such a scalability corresponds to the
 537 one observed for spheres by Zhao and Zhao (2019). Allocating more threads to
 538 the DEM simulation does not bring any benefit and can even be detrimental
 539 since parallel simulations using more 60 threads are eventually slower than the
 540 sequential one. This enhanced scalability of LS-DEM versus DEM relates with
 541 the former’s specificity that more than 99% of a sequential simulation is spent
 542 in contact treatment, with costly loops over boundary nodes.

543 6. Conclusions and perspectives

544 LS-DEM offers promising capabilities for arbitrary shape description in DEM
 545 with e.g. no inherent convexity requirements. Such a versatility requires a very
 546 significant amount of data per DE to be stored and numerically estimated during
 547 the DEM workflow, with three-dimensional tables of distance values on a grid,
 548 together with a set of boundary nodes for the purpose of master-slave contact

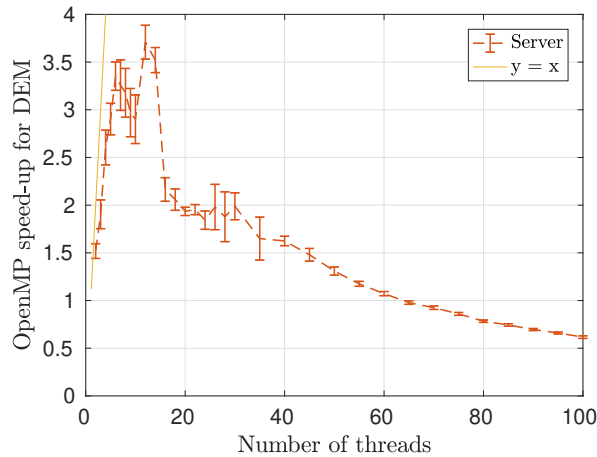


Figure 13: OpenMP speed up for the DEM triaxial compression on spheres

549 algorithms. By investigating simple configurations at the contact- and packing-
 550 scales for ideal spherical shapes with DEM serving as a reference, as well as
 551 superellipsoid ones, the precision of LS-DEM is shown to depend both on grid
 552 resolution and boundary nodes. On the present comparisons, reaching a good
 553 precision requires few tenths of grid spacings per particle size, as well as a couple
 554 of thousands boundary nodes.

555 Such choices dramatically increase computational costs of the simulations, be
 556 it in terms of memory (RAM) requirements or evaluation time. While sequential
 557 3D DEM simulations at the sample scale usually weigh hours and megabytes,
 558 LS-DEM requires days and gigabytes, after an implementation based onto the
 559 YADE code. Time costs nevertheless can be significantly decreased through par-
 560 allel computing with few tenths of threads, whereby a simple OpenMP frame-
 561 work decrease time costs by more than an order of magnitude.

562 Other parallel paradigms such as MPI, distributing memory instead of shar-
 563 ing it, may be even more useful and have yet to be investigated. Together with
 564 possible code and algorithmic (Duriez and Galusinski, 2020) improvements, they
 565 will hopefully make geotechnical simulations with real particle's shape even more
 566 affordable.

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