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A discrete-based multi-scale modeling approach for the propagation of seismic waves in soils

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Abstract

A three-dimensional multi-scale discrete-continuum model (Finite Volume Method \times Discrete Element Method, FVM \times DEM) is developed for a discrete-based description of the mechanical behavior of granular soils in boundary value problems (BVPs). In such a scheme, the constitutive response of the material is derived through direct DEM computations on a representative volume element attached to each mesh element. The developed multi-scale approach includes the inertial effect in the stress homogenization formulation and serves to study the mechanism of propagation of seismic waves, in comparison with a more classical BVP simulation that adopts an advanced bounding surface plasticity model "P2PSand". We start with a detailed and fair calibration and validation of these two models against laboratory tests for Toyoura sand under monotonic and cyclic loading. Then, the performance of the two approaches is compared for the case of a seismic wave loading passing through a saturated soil column with different relative densities, revealing several differences between the results of the two models.

Keywords: Multi-scale, DEM, Toyoura sand, seismic waves propagation, Bounding surface plasticity, inertial effect

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1. Introduction

Proper numerical simulations of cyclic and seismic loadings, including liquefaction phenomena, are an important issue for the safety of any earth structure. Different strategies can be used to simulate a soil seismic response numerically. First, classical elastoplastic constitutive models such as Mohr-Coulomb and Cam Clay (Roscoe and Burland, 1968) models can reproduce the monotonic behavior of different soils under drained and undrained conditions with different levels of precision. However, the features of these models are not rich enough to directly simulate the cyclic phenomena during seismic loading (e.g., the irrecoverable volumetric strains produced by cyclic loading are not taken into account). The first strategy for cyclic modeling involves using such simple models in conjunction with damping (hypoelasticity) (Woodward and Griffiths, 1996) and an ad-hoc relation that relates the increment of the plastic volumetric strain per cycle to the number of cycles by an empirical formulation as shown by (Martin et al., 1975; Byrne, 1991). This method is easy to implement and can provide an overall quantitative description of the cyclic response of soils but it cannot give an accurate description. Second, kinematic hardening is recognized as a fundamental element for reproducing the cyclic behavior of soils. Comprehensive and elaborated constitutive models such as DM04 (Dafalias et al., 2004), CJS (Duriez and Vincens, 2015), P2PSand (Cheng and Detournay, 2021) and numerous other approaches in Kutter et al. (2019) used the kinematic hardening to reproduce an evolving soil behavior during cyclic loading, being caused by microstructural hardening mechanisms such as an evolution of fabric. This feature allows the models to follow the degradation of the material during cyclic loading.

Finally, the DEM approach is shown to be able to reproduce most of the soil features during monotonic and cyclic loading (Mohamed et al., 2022; Sibille et al., 2019; Gu et al., 2020; Xie et al., 2022) including the liquefaction phenomenon by using three or four contact parameters at the interparticle level depending on shape descriptions. In principle, the DEM deals with the real

31 physics of granular media in which each particle is represented by its shape,
32 mass, and inertia so that it can be a robust technique for studying the be-
33 havior of soils under cyclic and dynamic loadings and can also address all the
34 shortcomings of phenomenological models that come from different hardening
35 mechanisms.

36 Recently, many publications have proposed the multi-scale approach (Kouznetsova
37 et al., 2002; Nguyen et al., 2014; Guo and Zhao, 2014; Nitka et al., 2009; Liu
38 et al., 2016; Kuhn, 2022) to describe soil behavior in a boundary value problem
39 (BVP) using information from the micro level via the discrete element method.
40 In essence, finite element or finite volume codes provide a numerical solution
41 for the differential equations for a continuous medium as seen at the BVP-scale.
42 At some point in the numerical scheme, i.e., before solving the equation of mo-
43 tion, a constitutive relation is required to present the internal stresses. To this
44 end, the constitutive response of the material is derived through direct DEM
45 computations on the representative elementary volume (REV) attached to each
46 Gauss point in the mesh without adding any empirical relationships.

47 In this study, we establish an information-passing coupling between a dis-
48 crete element and a finite volume continuum code by which the constitutive
49 response of the material is derived through direct DEM computations on a rep-
50 resentative elementary volume (REV) attached to each mesh zone. The two
51 codes used are: 1- FLAC3D (Itasca, 2019): a multi-dimensional Lagrangian
52 explicit finite volume program to study numerically the mechanical behavior of
53 a continuous three-dimensional medium (macro-scale). 2- PFC (Itasca, 2018):
54 a program that models the movement and interaction of stressed assemblies of
55 rigid particles with different shapes using the Distinct-Element Method (micro-
56 scale).

57 For the multi-scale modeling, the stress homogenization formulation for the
58 representative elementary volume REV is an essential element (Weber, 1966;
59 De Saxcé et al., 2004; Bagi, 2003). For this purpose, we review the definition of
60 the stress tensor for granular materials during dynamic events such as seismic
61 and shock loadings for proper inclusion of the effect of shear strain rate and

62 particle inertia on the mechanical behavior of granular media.

63 Then, we propose and discuss a multi-scale discrete-continuum modeling
64 approach for the propagation of seismic waves through a saturated soil column
65 made of Toyoura sand, a case study similar to the one by Taiebat et al. (2010)
66 and multi-scale FDM-DEM method proposed by Kuhn (2022), in comparison
67 with the direct use of an advanced elastoplastic model P2PSand (Cheng and De-
68 tournay, 2021; Itasca, 2019) in FLAC3D. It is worth noting our use of P2PSand
69 model relates with other previous studies using advanced elastoplastic consti-
70 tutive models in FLAC/FLAC3D to model wave propagation and liquefaction,
71 such as the SANISand (Yang et al., 2020) and UBCSAND (Tsiaousi et al.,
72 2020) models. Finally, we investigate the predictions of these two methods for
73 the occurrence of the so-called "dynamic liquefaction" for a loose soil column
74 after a fair quantitative calibration and validation process of the two numerical
75 approaches at the sample scale under monotonic and cyclic loadings.

76 The article consists of four main sections. Section 2 describes the P2PSand
77 constitutive model and its predictions for monotonic and cyclic loadings. Section
78 3 presents the DEM model previously developed by Mohamed et al. (2022) and
79 herein used in the multi-scale framework as well as its calibration and validation
80 for different monotonic and cyclic loading paths and points out the importance
81 of a proper stress homogenization formula for dynamic loadings. Section 4
82 discusses the multi-scale modeling implementation and presents the validation
83 of the latter when considering laboratory tests under different loading paths for
84 drained and undrained conditions. Section 5 shows and discusses the comparison
85 between the two approaches for the propagation of seismic waves as well as the
86 effects of the DEM damping and particle sizes on the response of the multi-scale
87 model.

88 **2. P2PSand constitutive model**

89 *2.1. Model overview*

90 The P2PSand model (practical two-surface plastic sand) has been developed
91 for general 3D geotechnical earthquake engineering applications by (Cheng and

92 Detournay, 2021; Itasca, 2019). The model follows critical state plasticity within
 93 a bounding surface framework (Dafalias et al., 2004) through the inclusion of a
 94 scalar state parameter (Been and Jefferies, 1985) for sand. The state parameter
 95 of the present model is chosen as the pressure ratio index I_p which is defined
 96 in the $D_r - p'$ as the ratio between the current mean pressure p' and the corre-
 97 sponding critical state mean pressure plane for the same relative density value
 98 D_r . The relative density is indeed used instead of the void ratio inside all the
 99 equations of the model because it is directly reachable from in-situ tests.

100 In the deviatoric plane π (Fig. 1), the elastic domain is limited by a small
 101 circular yield surface that does not change in size during loading (no isotropic
 102 hardening is allowed) with a kinematic hardening tensor $\boldsymbol{\alpha}$ which is the center
 103 of this circle. The yield surface is actually described by the same function as in
 104 DM04 model (Dafalias and Manzari, 2004):

$$f = [(\boldsymbol{s} - p\boldsymbol{\alpha}) : (\boldsymbol{s} - p\boldsymbol{\alpha})]^{0.5} - \sqrt{2/3}pm = 0 \quad (1)$$

105 Where m is the size of the yield surface and is used as a fixed value of $m =$
 106 $0.02M_{comp}$. M_{comp} is the critical-strength parameter for the triaxial compres-
 107 sion path. p is the effective mean stress (isotropic stress) and \boldsymbol{s} is the deviatoric
 108 stress tensor.

109 Besides the yield surface, the model incorporates four other surfaces in the
 110 normalized π plane as shown in Fig. 1. A constant critical state surface, bound-
 111 ing and dilatancy surfaces follow the same form as the bounding surface model
 112 proposed by Dafalias et al. (2004) with a Lode angle dependency. By shear-
 113 ing towards the critical state, the bounding and dilatancy surfaces evolve until
 114 they coincide with the critical state surface. In addition, an isotropic memory
 115 surface has the same shape as the bounding or dilatancy surface. Its size is
 116 determined by the historic position of $\boldsymbol{\alpha}$. The main purpose of this last surface
 117 is to avoid overshooting behavior during reversal loadings. Finally, the detailed
 118 formulations of the P2PSand model are given in Appendix A.

119 Table 1 presents the dimensionless parameters of the P2PSand model. The
 120 model adopts a unique critical state line that is defined based on the finding

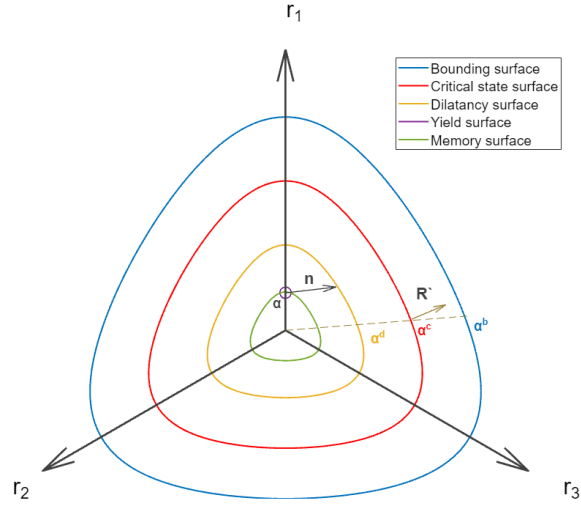


Figure 1: Schematic of different surfaces in the π plane for the P2PSand model after (Cheng and Detournay, 2021).

121 of Li and Wang (1998) with three parameters D_{rc0} , λ_c and ζ . While for the
 122 critical strength, the parameter c represents the ratio between extension and
 123 compression triaxial critical strengths. n_b and n_d are two model parameters
 124 that are used to determine the size of the bounding and dilatancy surfaces. The
 125 rate of plastic strains is controlled by two parameters, h_0 is the plastic shear
 126 rate and A_{d0} is the plastic volumetric rate. Also, the plastic volumetric rate is
 127 impacted by the evolution of fabric with an evolving rate depending on the C_z
 128 parameter until reaching maximum fabric magnitude z_{max} . The previous two
 129 parameters could be internally defined by the model or to be inserted directly
 130 by the user. Finally, K_{cyc} parameter intervenes when the state of the kinematic
 131 hardening tensor α is inside the memory surface in Fig. 2 to capture the sand
 132 behavior by which dilation/contraction evolution rate is lower during cyclic
 133 loading compared to virginal loading.

134 *2.2. Calibration and validation of the P2PSand model for different monotonic*
 135 *and cyclic loadings*

136 The essence of elastoplastic models is that strains are divided into elastic
 137 and plastic components and it can be considered that plastic deformations are

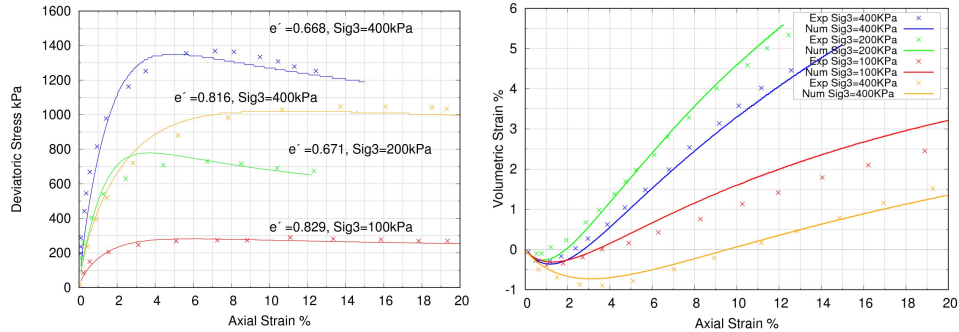


Figure 2: Results of P2PSand model for Toyoura sand along drained triaxial compression for various initial void ratios and initial mean pressure with one calibration test ($\sigma_3 = 400$ kPa and initial void ratio = 0.668) and three other validation tests. Experimental data from Fukushima and Tatsuoka (1984).

138 responsible for the evolution of pore pressure in undrained conditions and, as
 139 a result, for the loss of material strength in such conditions often encountered
 140 in practice. Therefore, the calibration of the elastoplastic models should be
 141 based on stress paths that make it possible to distinguish between the elastic
 142 and plastic strains e.g drained tests with several loading and unloading inter-
 143 mediate paths or undrained tests. Here, the calibration of the P2PSand model
 144 parameters for Toyoura sand (Table 1) is performed based on one drained and
 145 one undrained triaxial compression test. For this calibration phase, Fig. 2 re-
 146 presents the results of the P2PSand model together with experimental data from
 147 Fukushima and Tatsuoka (1984) for triaxial drained compression tests for var-
 148 ious initial void ratios and confining pressures. The model presents a close fit
 149 with the corresponding experimental results for the deviatoric stress and vol-
 150 umetric strain responses by introducing the effect of different initial void ratio
 151 values on mechanical behavior. During undrained tests, the model results are
 152 assessed for compression triaxial tests in Fig. 3 together with experimental data
 153 from Yoshimine et al. (1999). The results of the undrained compression tests
 154 can validate with good precision the experimental data.

155 Afterwards, the predictive abilities of the model under cyclic triaxial tests
 156 are evaluated. Actually, one parameter in Table 1 k_{cyc} should still be calibrated
 157 at this stage. Therefore, the model is calibrated for one cyclic test and validated

Table 1: P2PSand model dimensionless parameters for Toyoura sand with $D_r \in [0,1]$

Criteria	Parameter Symbol	Toyouira sand
Elastic-moduli	G_0	200
	C_{Dr}	0.8
	n	0.5
	ν	0.12
Critical state line	D_{rc0}	0.145
	λ_c	0.035
	ζ	0.7
Critical state surface	ϕ_{comp}	32°
	c	0.7
Bounding surface	n^b	0.13
Dilatancy surface	n^d	0.2
Hardening model	h_0	1.1
Dilatancy	A_{d0}	0.65
Fabric influence	C_z	$G_0(D_r + C_{Dr})$
	Z_{max}	$21D_r^{3.85} < 15$
Cyclic Loading	k_{Cyc}	0.4

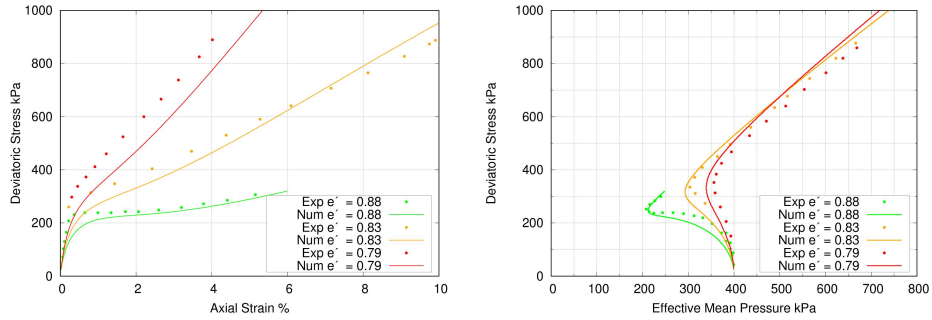


Figure 3: Results of P2PSand model for Toyoura sand along undrained triaxial compression for various void ratios with one calibration test $\sigma_3 = 400$ kPa and void ratio = 0.79 and two other validation tests. Experimental data from Yoshimine (2013).

158 for another cyclic test. Wang et al. (2016) provided the experimental data for
 159 Toyoura sand prepared using the air-pluviation method, which is consistent with
 160 the previous samples used by (Fukushima and Tatsuoka, 1984) for monotonic
 161 loadings. The experimental data are for different cyclic triaxial tests with differ-
 162 ent densities and cyclic stress ratios $CSR=q/2p_0$ (ratio between cyclic deviatoric
 163 stress amplitude and initial confining pressure) as shown in Fig. 4 and Fig. 5
 164 respectively. The results demonstrate that there are still some difficulties in fol-
 165 lowing the exact same evolution as the experimental data at the different stages
 166 of the test. Also, the P2PSand model shows a bias in the deviatoric stress vs
 167 axial strain curve by which the axial strain accumulates progressively on the
 168 extension side of the curve. Nevertheless, the model gives acceptable predic-
 169 tions in terms of the number of cycles required to reach liquefaction (i.e., zero
 170 mean effective stress) and liquefaction phenomena simulation (the progressive
 171 decrease in effective mean pressure and the butterfly shape) compared to the
 172 experimental data. Indeed, for these two tests with $CSR=0.147$ and 0.163 the
 173 numbers of cycles required to attain an axial strain value of about $\epsilon_a=9\%$ are
 174 ($N_{Exp} = 37, N_{P2PSand} = 32$) and ($N_{Exp} = 12, N_{P2PSand} = 17$) respectively.

175 **3. 3D-DEM model for Toyoura sand**

176 *3.1. Model formulation and generation procedure*

177 A DEM model for Toyoura sand previously presented in (Mohamed et al.,
 178 2022) is used. It includes a constant-stiffness rolling resistance contact model
 179 with 4 parameters and spherical particles that follow the same particle size
 180 distribution as Toyoura sand as shown in Fig. 6 (model 1) except for a scaling
 181 factor that was mechanically inconsequential by virtue of the contact model in
 182 the quasi-static cases. However, in the present context where dynamic effects are
 183 anticipated to take place, we also consider the exact granular size distribution
 184 as shown in Fig. 6 (model 2, differing from model 1 only in that aspect).

185 DEM samples are created by starting with a cloud of non-overlapped par-
 186 ticles within rectangular parallelepiped rigid walls. The walls are then moved
 187 inwards in order to reach a target compaction pressure. A 3D-DEM REV with

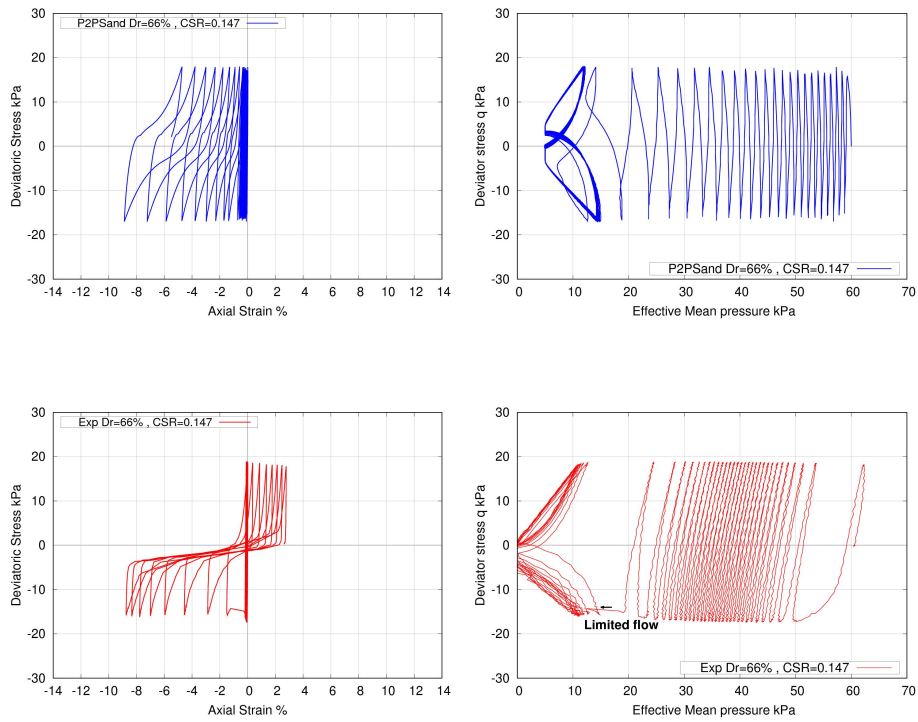


Figure 4: (Top) Results of the P2PSand model for an undrained cyclic triaxial test for Toyoura sand sample with $D_r = 66\%$ and $CSR=0.147$ serving as calibration. (Bottom) Experimental data from Wang et al. (2016).

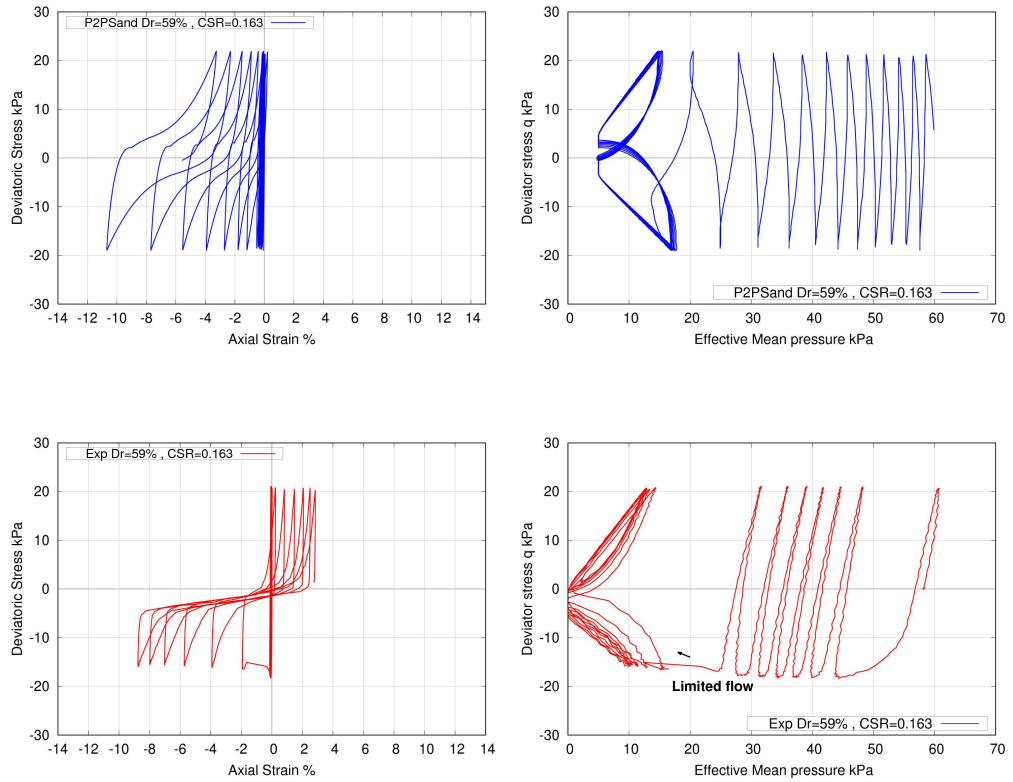


Figure 5: (Top) Results of the P2PSand model in a validation stage for an undrained cyclic triaxial test for the Toyoura sand sample with $D_r = 59\%$ and $CSR = 0.163$. (Bottom) Experimental data from Wang et al. (2016).

188 a number of $N_b=7000$ particles is used for the current multi-scale modeling of
 189 Toyoura sand, as it was proven by Mohamed et al. (2022) that this number is
 190 sufficient to give a homogeneous distribution of the void ratio inside the sample
 191 and an unaffected stress-strain response when the number of particles exceeds
 192 this value. It is worth mentioning that considered DEM samples always show
 193 the same initial void ratio values as the reference lab experiments. Reaching
 194 such given initial void ratio values is achieved during that compaction phase
 195 based on the friction coefficient and rolling coefficient values, which are tuned
 196 independently of the subsequent shear loading phase. The contact parameters
 197 and packing properties, including a zero initial anisotropy due to the isotropic
 198 generation, are summarized in Table 2. The corresponding DEM and P2PSand
 199 relative density values are calculated based on the maximum and minimum void
 200 ratio values $e_{min} = 0.6$ and $e_{max} = 1$ of Toyoura sand.

201 Following Mohamed et al. (2022) who provided a detailed presentation, the
 202 rolling resistance contact model with 4 contact parameters is used as shown in
 203 Table 2, where E_{mod} , K_n , K_s are effective modulus i.e. the constant normal
 204 stiffness scaled with respect to (divided by) particle size, the actual normal
 205 stiffness and its tangential counterpart. The friction μ and rolling friction μ_r
 coefficients are imposed on the contact to limit shear force and moment.

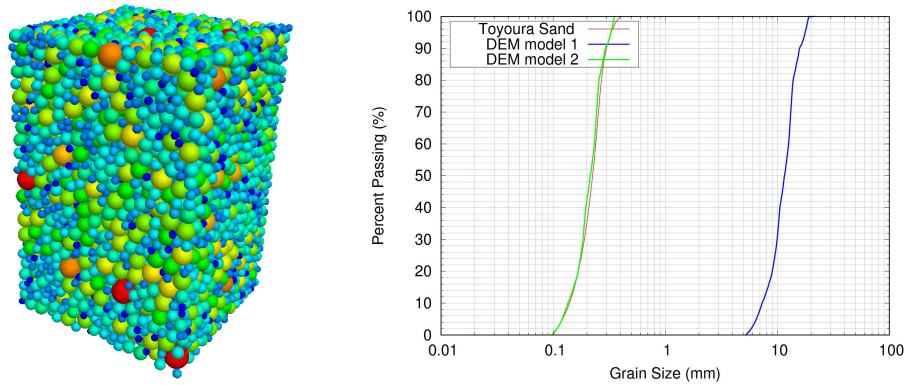


Figure 6: Left: Toyoura sand 3D-DEM model where different colors refer to different diameters. Right: different particle size distributions for DEM (model 1 and model 2) vs Toyoura sand from Dong et al. (2016)

206

Table 2: 3D-DEM model parameters for different DEM and multi-scale simulations

Contact				Packing (see also Fig. 6 for psd)			
E_{mod} (MPa)	K_n/K_s (-)	μ (-)	μ_r (-)	N_b (-)	Initial anisotropy	Grain mass density (kg/m^3)	Relative density (%)
400	3	0.6	0.38	7000	Variable (0 for lab tests)	2600	Variable

207 *3.2. Calibration and validation of the 3D-DEM model for monotonic loadings*

208 The calibration of the used DEM model for Toyoura sand was performed
 209 in (Mohamed et al., 2022) based on a drained triaxial test. During the valida-
 210 tion process, the model was therein validated to fit other experimental data of
 211 drained and undrained triaxial tests (compression and extension). The results
 212 of the drained triaxial tests were in good accord with the corresponding ex-
 213 perimental data for the different triaxial compression tests with different initial
 214 void ratio values. One may note that during the undrained extension triaxial
 215 tests, the model showed less ability to lose effective strength when compared to
 216 the experimental data, unlike another polyhedra-based model also proposed in
 217 (Mohamed et al., 2022). However, we stick here to the sphere-based model due
 218 to the computational costs of multi-scale simulations.

219 *3.3. Validation of the DEM model under cyclic loading*

220 In line with the present focus on seismic loadings, the predictions of the
 221 DEM model for different undrained cyclic tests are herein investigated. The
 222 predictions of the DEM approach and two experimental data for two undrained
 223 cyclic triaxial tests Wang et al. (2016) with different values of $CSR = 0.147$
 224 and 0.163 and initial $p' = 60$ kPa are shown in Fig. 7 and 8. For these two
 225 tests with $CSR=0.147$ and 0.163 the number of cycles required to attain an
 226 axial strain value of about $\epsilon_a = 9\%$ is ($N_{Exp} = 37, N_{DEM} = 40$) and ($N_{Exp} =$
 227 $12, N_{DEM} = 20$) respectively. Compared to monotonic loadings, less accurate
 228 predictions are observed compared with the experimental data since the initial
 229 plastic flow is initiated on the compression side, which may be attributed to
 230 different initial fabric anisotropies when compared to the experimental data.
 231 Nevertheless, the DEM model gives satisfactory results since it doesn't exhibit

232 the illogical behavior that was observed previously by using the P2PSand model,
 233 particularly the evolution in one direction in the deviatoric vs axial strain $q - \epsilon_a$
 234 plane, the discontinuity in $q - \epsilon_a$ and deviatoric stress vs effective mean pressure
 $q - p'$ planes and the non-occurrence of limited flow before liquefaction.

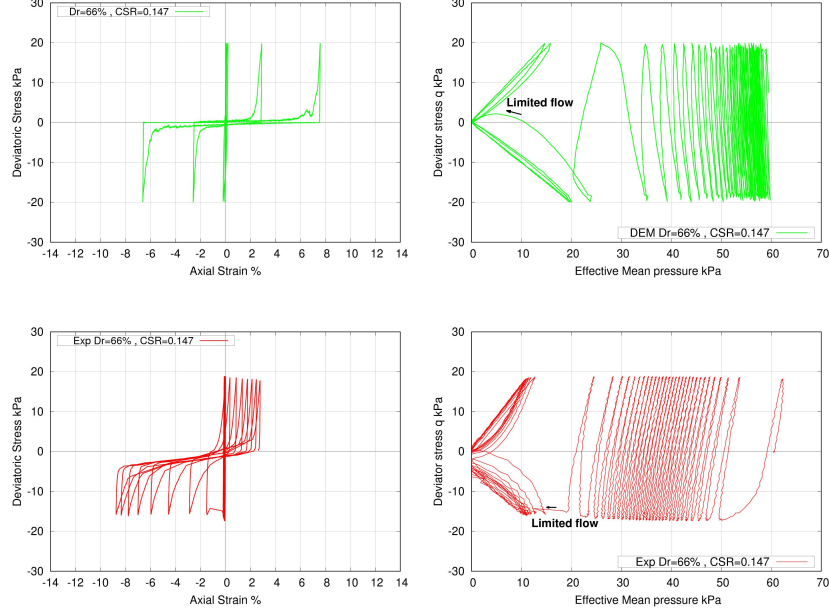


Figure 7: Deviatoric stress versus axial strain and effective pressure in undrained cyclic triaxial tests of Toyoura sand, with initial $p'=60$ kPa and $Dr=0.66$, $CSR=0.147$ — comparison of DEM results (solid green) with experimental data from Wang et al. (2016) (solid red).

235

236 3.4. Review of homogenization formulas for the stress tensor of a DEM packing 237 including dynamic effects

238 To make a step from micro- to macro-scale, the REV stress response is
 239 computed using the stress homogenization formula (Weber, 1966; Christoffersen
 240 et al., 1981) for the static part contribution of a stressed particle assembly as
 241 follows:

$$\sigma^W = -\frac{1}{V} \sum_{N_c} \mathbf{F}^{(c)} \otimes \mathbf{L}^{(c)} \quad (2)$$

242 where V and N_c are the packing volume and the number of contacts inside that
 243 volume respectively. $\mathbf{F}^{(c)}$ and $\mathbf{L}^{(c)}$ represent the contact force and branch vector

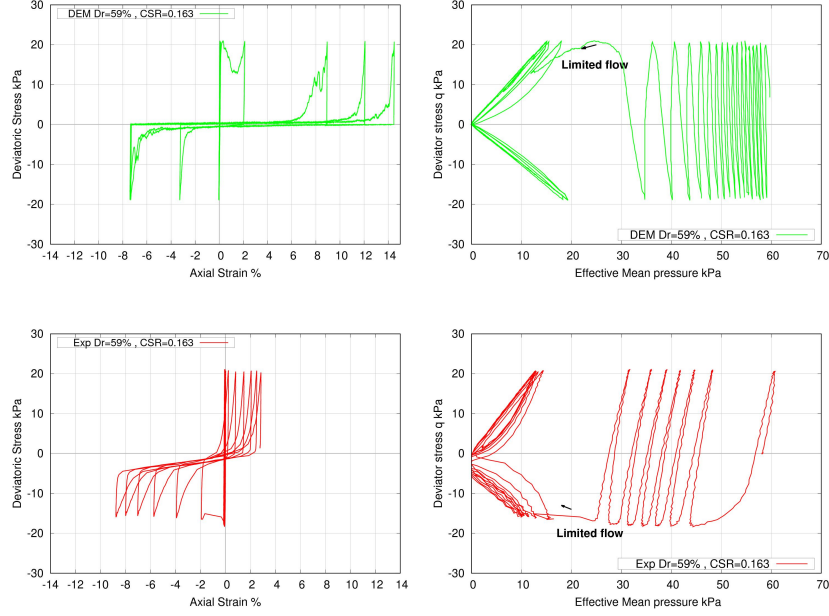


Figure 8: Deviatoric stress versus axial strain and effective mean pressure in undrained cyclic triaxial tests of Toyoura sand, with initial $p'=60$ kPa and $Dr=59\%$, $CSR=0.163$ — comparison of DEM results (solid green) with experimental data from Wang et al. (2016) (solid red).

244 respectively.

245 As highlighted by (Yan and Regueiro, 2019; Duriez and Wan, 2017), the
 246 effect of boundary contacts cannot be neglected for a relatively small number of
 247 particles in REV. Bagi (2003) proposed a stress tensor formula that takes into
 248 account the external contact forces as follows:

$$\sigma^B = -\frac{1}{V} \left(\sum_{N_c} \mathbf{F}^{(c)} \otimes \mathbf{L}^{(c)} + \sum_{N \in E} \mathbf{F}^{(N)} \otimes \mathbf{L}^{(N)} \right) \quad (3)$$

249 where E denotes particle contacts that lie on the boundary of the REV and
 250 $\mathbf{L}^{(N)}$ is the branch vector of the external contact point.

251 The applications of the current multi-scale modeling are oriented to seismic
 252 analysis where dynamic effects i.e., inertial terms, should not be neglected.
 253 De Saxcé et al. (2004) take into account those inertial terms, together with the
 254 effect of body forces, as follows:

$$\boldsymbol{\sigma}^D = -\frac{1}{V} \left(\sum_{N_c} \mathbf{F}^{(c)} \otimes \mathbf{x}^{(c)} + \sum_{N \in E} \mathbf{F}^{(N)} \otimes \mathbf{L}^{(N)} + \int_V \rho \mathbf{x} \otimes (\mathbf{g} - \mathbf{a}) dV \right) \quad (4)$$

255 where \mathbf{x} denotes the spatial coordinates while ρ , \mathbf{g} and \mathbf{a} are mass density,
 256 gravitational and inertial accelerations respectively. For the present multi-scale
 257 simulations where materials may be subjected to severe dynamic actions i.e.,
 258 earthquakes and impact loadings, the stress tensor formula in Eq. 4 is adopted,
 259 as justified below.

260 3.5. Numerical investigation of inertial effect

261 The purpose of this section is to check the previous homogenization equation
 262 by considering one example where dynamic effects occur. Five triaxial drained
 263 tests are performed with different strain rate values and shown in Fig. 9, cor-
 264 responding to different values of inertial number I as defined by Da Cruz et al.
 265 (2005):

$$I = \frac{\dot{\epsilon}_a D}{\sqrt{\frac{p'}{\rho}}} \quad (5)$$

266 where $\dot{\epsilon}_a$ is the axial strain rate, D the average particle diameter, p' is the
 267 effective pressure and ρ is the density. The DEM model 2 in Fig. 6 is utilized and
 268 the details of the numerical parameters are shown in Table 2. First, in Fig. 9 the
 269 contribution of each term of the stress tensor is investigated in order to examine
 270 how dynamic effects may influence and modify the average stress tensor. The
 271 deviatoric stress is calculated in two different ways, first, from the average stress
 272 values of the pair of boundary walls along each direction, and second, from the
 273 stress homogenization formula in Eq. 4. The results highlight the importance of
 274 the inertial part in Eq. 4 and show a significant difference between the static and
 275 dynamic definitions of stress tensors for the case of the most dynamic loading.
 276 In a second analysis in Fig. 10 showing the macroscopic sample behavior for
 277 all cases, one can see that, by increasing the inertial number of the simulation,
 278 the apparent modulus and deviatoric stress increase significantly, resulting in a
 279 more dilative response. In addition, no stable critical state can be achieved for

280 the most dynamic case ($I \in [4 \times 10^{-2}; 10^{-1}]$). Finally, while the three tests with
 281 the lowest strain rate values ($I < 2 \times 10^{-2}$) have very similar overall responses
 282 in the $q - \epsilon_a$ and $\epsilon_v - \epsilon_a$ curves, it should be noted that, as shown in Fig. 10,
 283 changing the inertial number in that interval still has a significant impact on
 284 the apparent modulus at the initial stage of these tests and that being closer to
 285 a quasi-static regime requires $I \approx 10^{-3}$.

286 These values are coherent with those of Da Cruz et al. (2005) who demon-
 287 strated that a quasi-static critical state regime with almost no variation in the
 288 effective friction coefficient requires very low values of $I=10^{-3}$ and that a fully
 289 collisional flow regime occurs for $I=10^{-1}$.

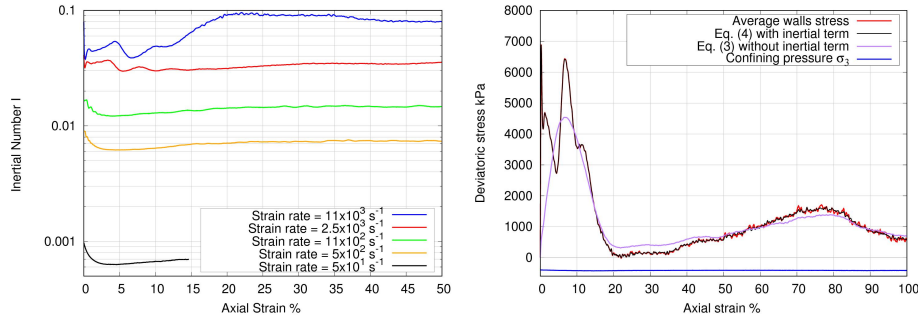


Figure 9: Left: inertial number during five different drained triaxial tests ($\sigma_3 = 400$ kPa and initial $n = 0.388$) with different values of strain rate. Right: Inertial term effect on deviatoric stress vs axial strain curve for strain rate = $11 \times 10^3 \text{ s}^{-1}$.

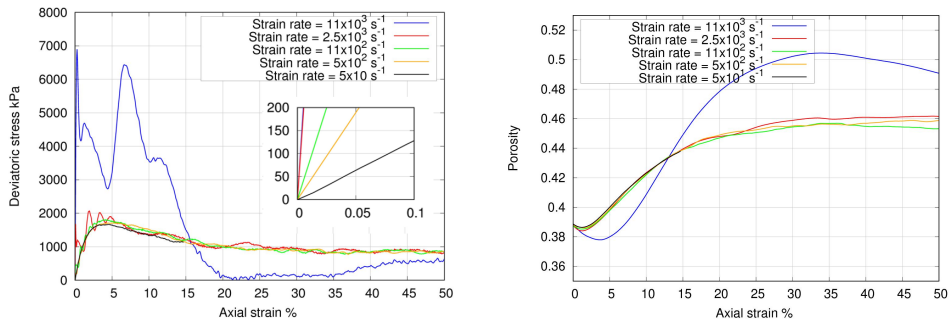


Figure 10: The effect of various strain rates and inertial number values on the macroscopic behavior of a drained triaxial test with $\sigma_3 = 400$ kPa and initial $n = 0.388$ enclosing a magnified scale for the initial part of the deviatoric curve for the different tests.

290 4. Multi-scale coupling method

291 4.1. Flac3D continuum model

292 The continuum medium in Flac3D is discretized into constant strain-rate
293 elements with a tetrahedral shape. The general numerical scheme is shown in
294 Fig. 11. At the beginning of each time step, the strain rate tensor $\dot{\epsilon}$ is defined
295 from nodal velocities. Then a constitutive relation is applied to define the new
296 stress tensor σ . Finally, the equation of motion is applied to compute the new
297 nodal velocities and therefore the new nodal displacement. The finite volume
298 formulation of Flac3D is presented in detail in Appendix B.

299 4.2. Multi-scale coupling of Flac3D and PFC

300 In this section, a two-scale numerical homogenization approach by FVM \times DEM
301 (in Flac3D and PFC software) is presented. Simultaneous running and compu-
302 tation are performed by these two codes. A unique DEM packing is assigned
303 as a REV bounded with rigid walls for each zone of Flac3D and the strain rate
304 tensor of each Flac3D zone is applied to each corresponding REV. Mainly, a
305 new plug-in c++ constitutive model is constructed in Flac3D to invoke a PFC
306 computation and to offer the new stress state to the Flac3D continuum model at
307 each timestep. In the present context between Flac3D and PFC, the strain rate
308 tensor $\dot{\epsilon}$ is conserved and not only the strain increment $d\epsilon$ to take into account
309 the inertial and viscous effects (if a viscous contact model would be applied) in
310 the behavior of granular mass (Jop et al., 2006).

311 Fig 11 shows the computational homogenization scheme applied to each time
312 step. It is worth noting that unlike coupling of DEM with the finite element
313 method (FEM \times DEM, Nguyen et al., 2017), the present scheme does not need
314 to establish a consistent tangent stiffness matrix from a DEM computation and
315 it is enough to update the stress matrix in the continuum model at each time
316 step based on the DEM computations.

317 Finally, the 3D-DEM REV presented previously in Section 3 with a number
318 of 7000 particles is used for the current multi-scale modeling of Toyoura sand, as

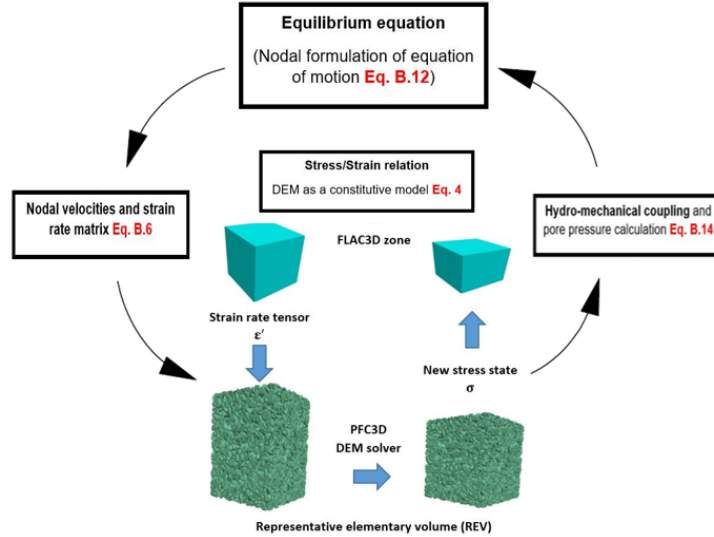


Figure 11: General Flac3D cycle in black and computational homogenization scheme Flac3D-PFC inset in color.

319 it was proven by Mohamed et al. (2022) that it is sufficient to give an unaffected
 320 stress-strain response when the number of particles exceeds this value.

321 *4.3. Validation of the multi-scale implementation under drained-undrained tri-*
 322 *axial and simple shear tests for Toyoura sand*

323 A verification procedure is first introduced on very simple cases with 1 or
 324 2 adjacent zones to check the correct implementation of the DEM–FVM cou-
 325 pling scheme. The predictions of corresponding Flac3D models for drained and
 326 undrained triaxial tests for loose and dense samples are tested. Fig. 12(a)
 327 shows the macroscopic response of a dense Toyoura sand sample ($D_r = 90\%$)
 328 until reaching the critical state condition. The results demonstrate stable nu-
 329 merical results at the different stages of the test (including the strain softening
 330 regime) until the critical state. In addition, the macroscopic response of each
 331 zone is shown to be identical to the corresponding REV response. As for the
 332 loose sample, a similar simulation is performed to check the numerical stability
 333 of the scheme for a case where more grain rearrangement and plastic deforma-
 334 tion are anticipated to take place. Fig. 12(b) shows the results of a triaxial

335 test for a relatively loose Toyoura sand sample $D_r = 40\%$. The results again
 336 confirm the stability of the coupling scheme for the deviatoric and volumetric
 337 strain curves.

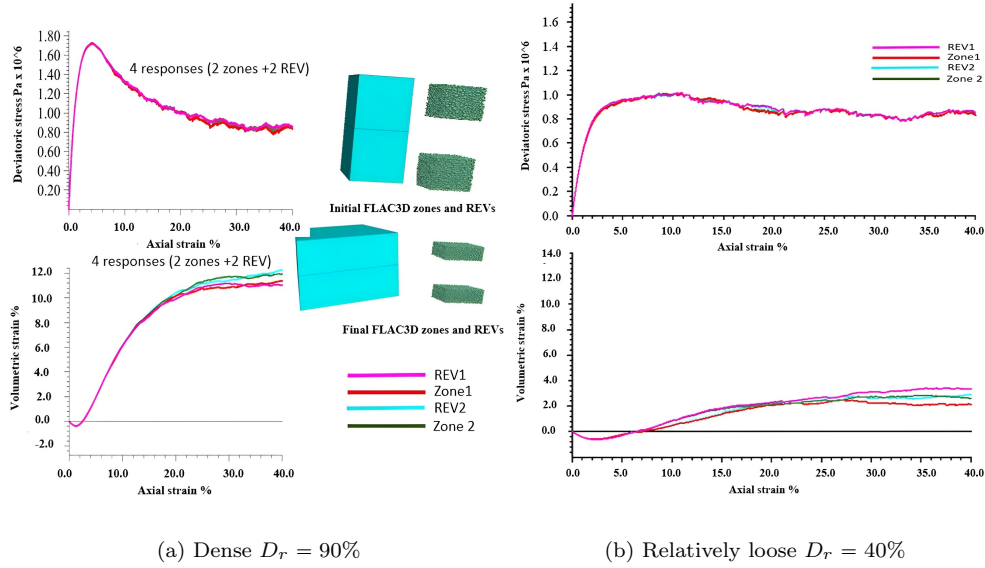


Figure 12: Deviatoric stress vs axial strain and volumetric strain vs axial strain for Toyoura sand with initial confining pressure = 400 kPa and two different initial porosity values.

338 Furthermore, a hydro-mechanical analysis is considered for an undrained
 339 triaxial test condition and is imposed in the Flac3D model where the pore pres-
 340 sure is generated due to the mechanical volumetric deformation and given water
 341 compressibility $k_f = 2$ GPa and $\alpha_{Biot} = 1$ (see Itasca (2019) and Appendix B)
 342 in a classical simplified version of the pore pressure update method proposed by
 343 Kuhn and Daouadji (2020). The results of the multi-scale model are shown in
 344 Fig 13 for an undrained condition for a loose sample with an initial confining
 345 pressure = 400 kPa. Results show almost similar responses for the undrained
 346 test using only the DEM and constant volume boundary condition presented in
 347 Mohamed et al. (2022). Also, a unique behavior is observed for the REV1s and
 348 Flac zones until a large axial strain value $\epsilon_a = 22\%$.

349 Finally, it is checked that the present use of rigid boundaries does not pre-

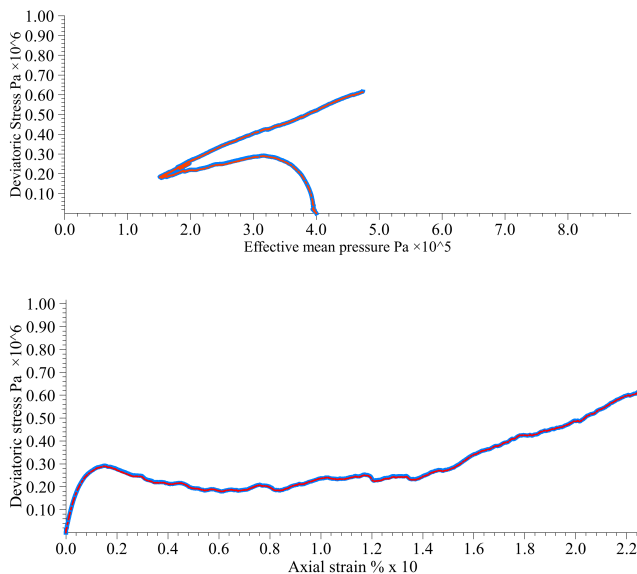


Figure 13: Deviatoric stress vs axial strain and effective mean pressure for a loose Toyoura sand sample ($D_r = 25\%$) during an undrained triaxial test with an initial confining stress=400kPa. The responses of DEM (red) and Flac upper zone (blue) are identical.

350 clude correctly addressing non-axisymmetric simulations such as simple shear.
 351 Duriez et al. (2011) actually suggested with a similar DEM setup that possible
 352 localization bias was absent until a significant shear strain value $\gamma=0.5$, in spite
 353 of the rigid boundaries. Here, the coupling scheme is assessed for a simple shear
 354 test with a single zone in Fig. 14, under an initial isotropic stress of 400 kPa, a
 355 constant $\sigma_{zz} = 400$ kPa and an initial porosity value of $n=0.41$. The REV and
 356 Flac zone give identical results until a large value of shear strain $\gamma = 0.65$.

357 5. Multi-scale modeling of seismic wave propagation through a satu- 358 rated soil column

359 5.1. Comparison of results from the multi-scale approach with the P2PSand- 360 based classical approach

361 As the main application, a vertical column of saturated sand made up of
 362 ten 3D zones is considered to be shaken by an earthquake as shown in Fig. 15.
 363 The sandy material is described either with the DEM or the P2PSand models
 364 described in the previous sections. Before the application of the earthquake

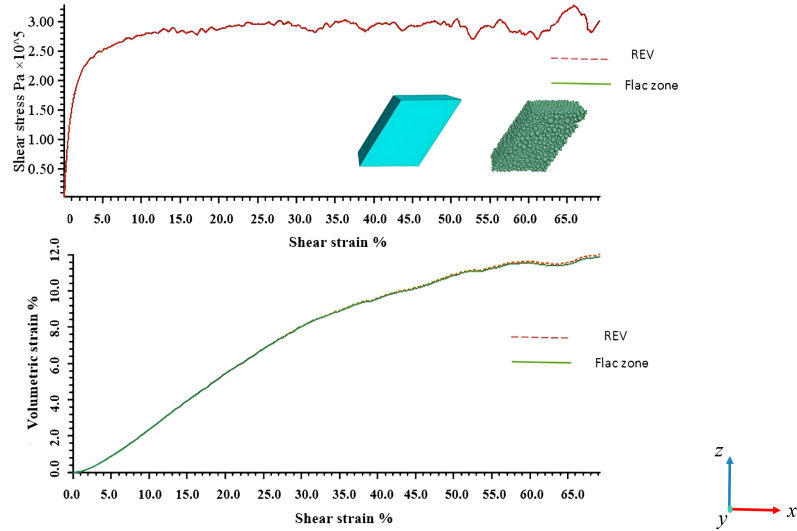


Figure 14: Simple shear test (constant σ_{zz}) with an initial isotropic stress of 400 kPa and an initial porosity value $n=0.41$.

365 wave, stresses are initialized to $\sigma_x = \sigma_y = 0.5\sigma_z$ inducing an initial anisotropic
 366 stress state all along the column. As with the previous undrained test, the pore
 367 pressure evolves throughout the fully saturated column in Flac3D only due to the
 368 mechanical volumetric change resulting from the seismic shaking. It is indeed
 369 assumed for simplicity that the characteristic time of the earthquake event is
 370 faster than the time required for the fluid to flow from one zone to another and
 371 Darcy's law and its diffusive effects are accordingly deactivated herein, even
 372 though a full hydro-mechanical coupling is technically possible in FLAC3D. The
 373 bedrock boundary condition is used at the bottom of the model and a constant
 374 lateral total stress is applied as a lateral boundary condition. In the case of
 375 using the P2PSand model, a 2% Rayleigh damping was employed while for the
 376 multi-scale model, a classical Cundall, i.e. global, damping (Cundall, 1987) with
 377 a 0.6 coefficient is used by default in the DEM, before being investigated in more
 378 detail in a forthcoming section. The earthquake loading is chosen as the Gilroy
 379 No.1 record of the 1989 Loma Prieta earthquake (which occurred on California's
 380 central coast), scaled to have a peak ground acceleration of 0.8 g in Fig. 15.

381 In order to analyze the models' response in light of the previous predictions of
 382 the models for cyclic triaxial tests (compression/extension) in Sections 2.2 and
 383 3.3, it is chosen to apply the input acceleration at the bottom as a P-wave.
 384 The simulations are performed for two cases with different initial density values
 385 representing the relatively dense and loose states of Toyoura sand. The results of
 386 the comparison between the two models during the shaking phase for both cases
 387 are analyzed in terms of stress-strain responses and acceleration time history at
 388 different levels of the column.

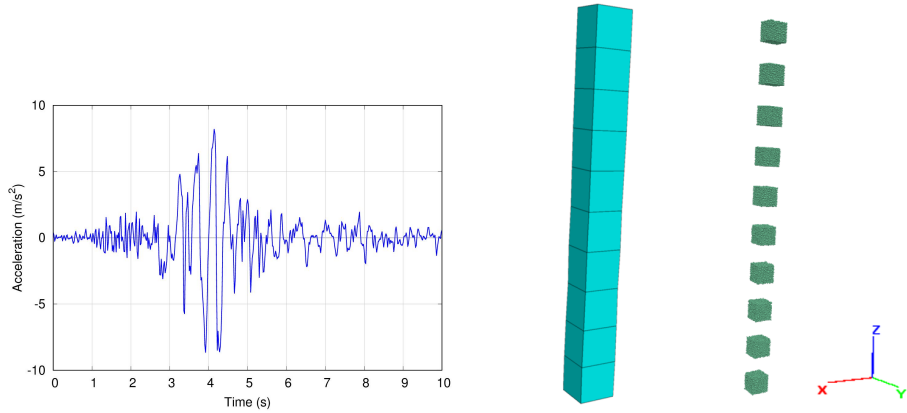


Figure 15: Left: The input vertical acceleration at the bottom zone. Right: the geometry of the Flac3D soil column and the corresponding REV's for multi-scale modeling.

389 Fig. 16 and Fig. 17 show the response of the soil column to the relatively
 390 dense soil $D_r = 60\%$ in terms of deviatoric stress vs axial strain and deviatoric
 391 stress vs effective mean pressure for the two models. As for the multi-scale,
 392 at the early stage of the shaking, an increase in the effective mean pressure is
 393 observed at the different levels due to the dilative tendency of the soil. However,
 394 later and during the intense waves, a slight decrease in the effective mean pres-
 395 sure is observed, coinciding with an accumulation of shear strains in all levels of
 396 the soil column, especially in the top zone. On the other hand, the response of
 397 the P2PSand model shows less ability to lose effective mean pressure and more
 398 tendency to accumulate axial strain only in the positive side (axial shortening)
 399 of the deviatoric stress vs axial strain curve.

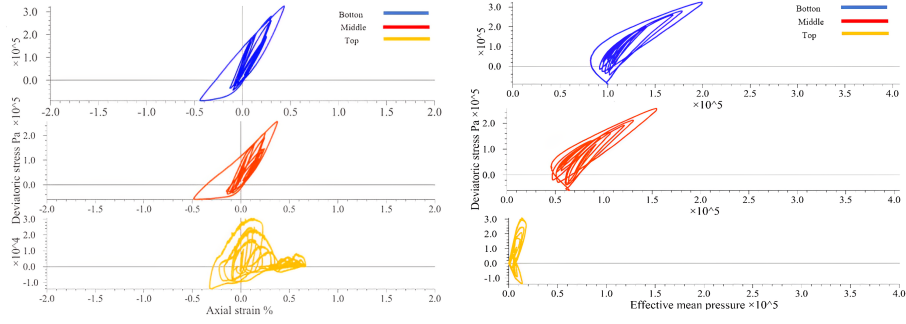


Figure 16: Multi-scale model predictions for a relatively dense soil column ($D_r = 60\%$). Left: deviatoric response at different positions of the soil column. Right: deviatoric stress vs effective mean pressure.

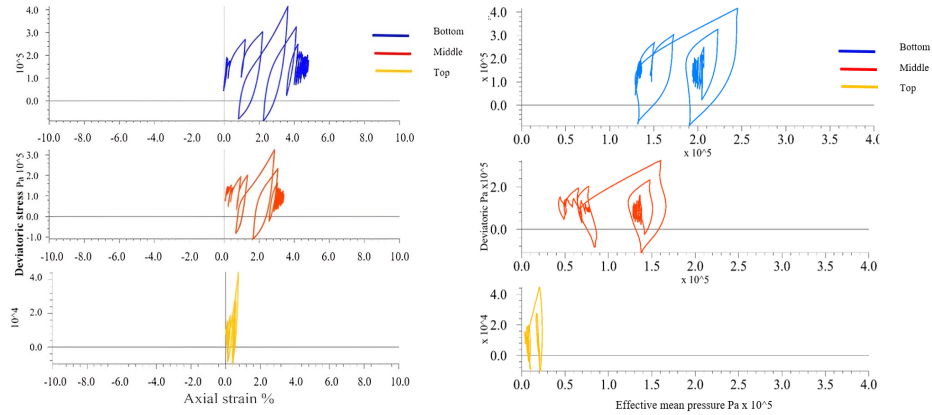


Figure 17: P2PSand model predictions for a relatively dense soil column ($D_r = 60\%$). Left: deviatoric response at different positions of the soil column. Right: deviatoric stress vs effective mean pressure.

400 The acceleration history is monitored at different levels and shown in Fig.
 401 18. Results show that the base acceleration is transmitted to the surface of the
 402 soil column in two models, resulting in a large amplitude at the surface of the
 403 soil. The two models exhibit almost the same maximum acceleration at the
 404 bottom and middle zones, but a larger acceleration at the top zone is observed
 405 for the P2PSand model compared to the multi-scale model.

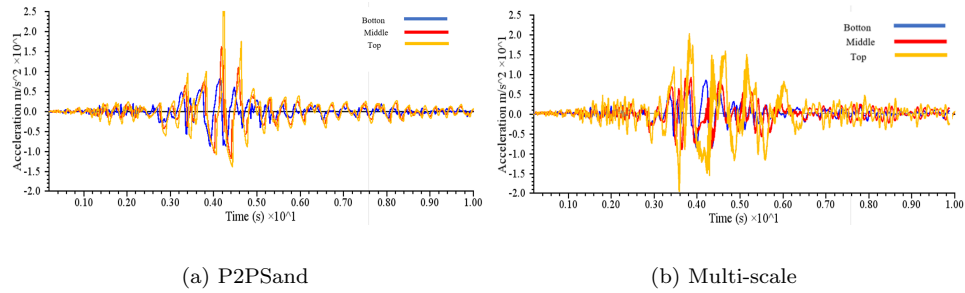


Figure 18: Acceleration time history for the P2PSand and Multi-scale models at different positions for a dense soil column of Toyoura sand.

406 The second case investigated is for a loose soil column with a relative density
 407 of $D_r = 25\%$. The results of the two models are shown in Fig. 19 and Fig.
 408 20. Despite the larger shear strain values observed for the P2PSand model
 409 in the bottom and middle zones as shown in Fig. 21, the results show that
 410 the liquefaction mechanism is also observed for the multi-scale model since the
 411 middle and top zones reach a zero effective mean pressure value during the
 412 event. In addition, the top zone of the multi-scale model shows higher axial
 413 and shear strains with $\epsilon_a \approx 4\%$, $\gamma \approx 6\%$ compared to the P2PSand model
 414 $\epsilon_a \approx 1.15\%$, $\gamma \approx 1.72\%$. Thinking of another, strain-based, liquefaction criterion
 415 such as proposed by Cappellaro et al. (2021) in terms of double-amplitude shear
 416 strain value $\gamma = 7.5\%$, one can note that this value that is not attained by the
 417 two models.

418 The acceleration responses for the loose case are shown in Fig. 22. The
 419 results of the two models are similar for the bottom and middle zones. However,
 420 more spike values are observed in the case of the multi-scale model at the top

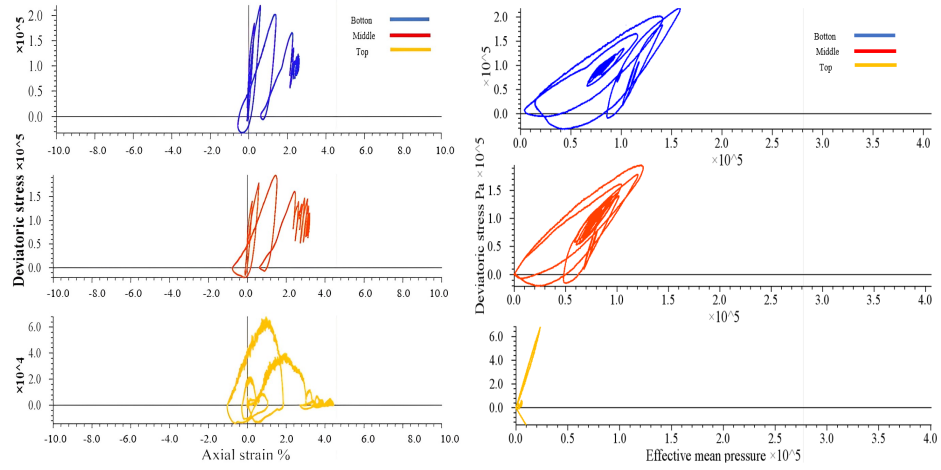


Figure 19: Multi-scale model predictions for a loose soil column ($D_r = 25\%$). Right: deviatoric stress vs effective mean pressure. Left: deviatoric response at different positions of the soil column.

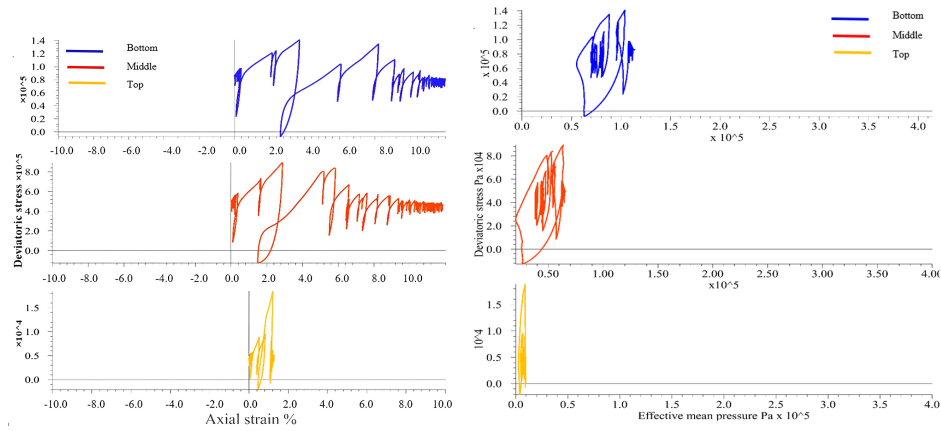


Figure 20: P2PSand model predictions for a loose soil column ($D_r = 25\%$). Left: deviatoric response at different positions of the soil column. Right: deviatoric stress vs effective mean pressure.

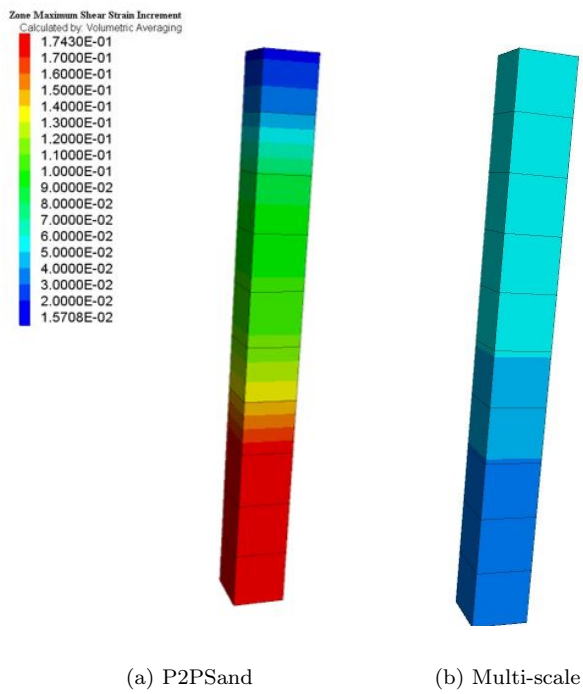


Figure 21: Shear strain profile along the soil column at $T=10$ s for the P2PSand and Multi-scale models for a loose soil column ($D_r = 25\%$).

421 zone due to the large deformation of this zone.

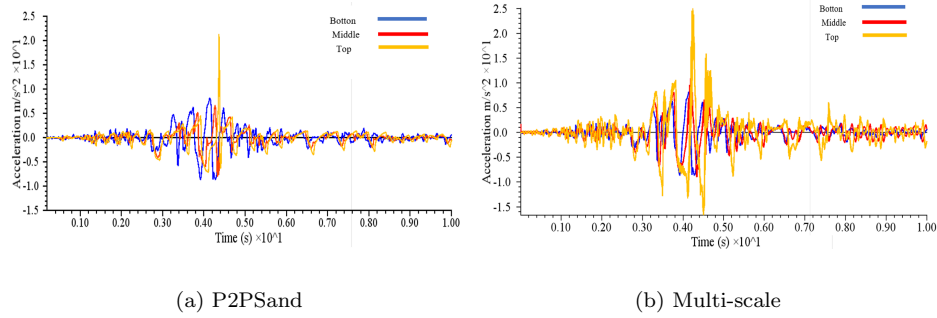


Figure 22: Acceleration time history for the P2PSand and Multi-scale models at different positions for a loose soil column of Toyoura sand.

422 In general, a clear contradiction is observed between the predictions of the
 423 two approaches since the large deformation occurs in the case of the multi-scale
 424 approach for the top zone, while the P2PSand model predicts a large deformation
 425 for the bottom zone. In addition, for the two studied relative density values,
 426 the multi-scale model gives lower axial strain at different positions, except for
 427 the top zone in the case of the loose case. Additionally, for the loose case, the
 428 multi-scale model shows acceleration amplification (Fig. 22) at the top zone
 429 when compared with the P2PSand model.

430 In addition to the macroscopic results, useful microstructure information can
 431 be elicited from the multi-scale model. Fig. 23 shows the evolution of the force
 432 networks for the loose soil column before and after the seismic event. Before the
 433 event, the vertical components of the force networks have the highest contact
 434 force, which is consistent with the initial anisotropic state of the samples. After
 435 the event, the top sample has a very weak force network due to liquefaction
 436 occurrence in this zone.

437 5.2. Parametric study on the damping coefficient and particle size

438 As for the multi-scale model, physically dissipative microscale phenomena
 439 such as contact friction serve as the main source of energy dissipation. As it is
 440 customary in DEM, a numerical Cundall damping is also herein present and may

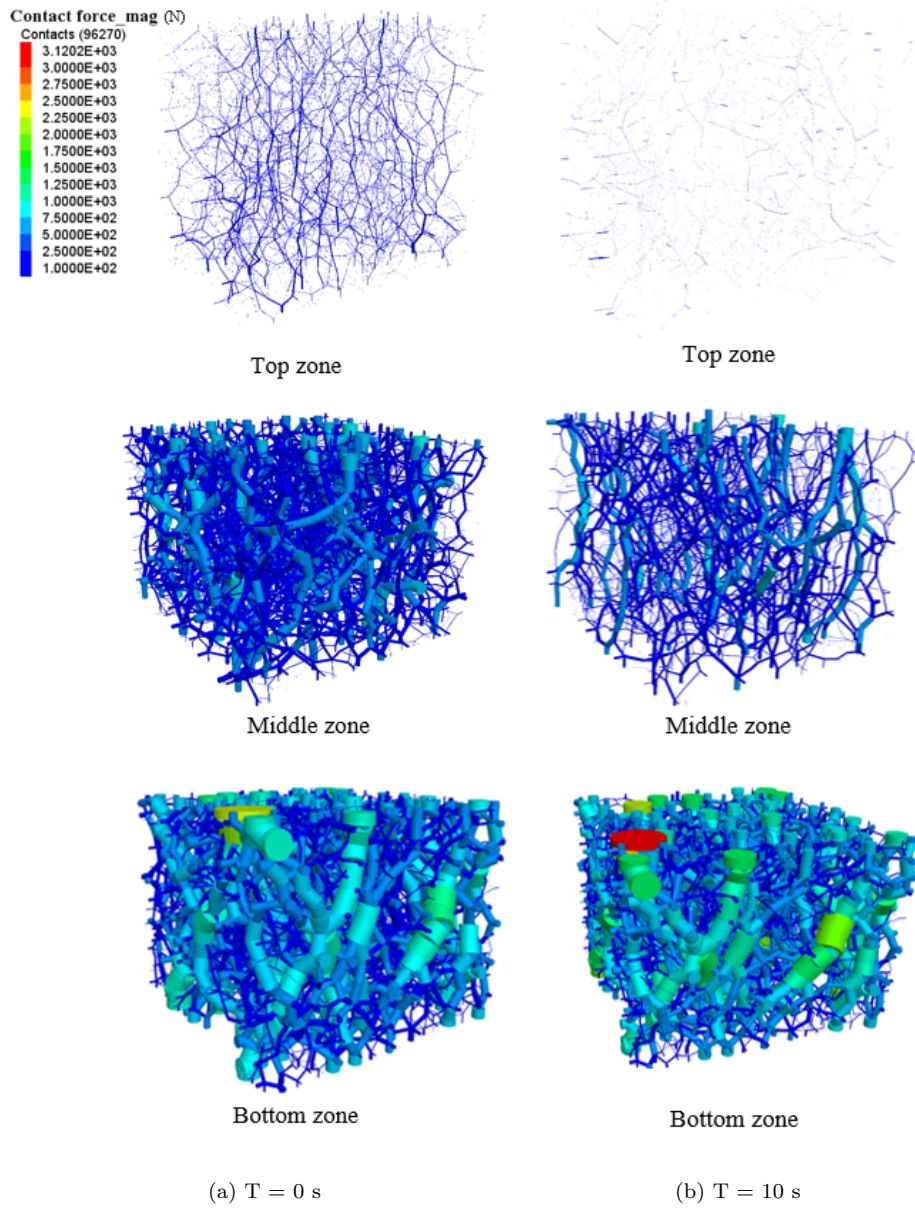


Figure 23: Force networks for different zones before and after the seismic event for the loose soil column.

441 artificially dissipate energy similar to the Rayleigh damping, which is employed
 442 in conjunction with the case of the continuum constitutive model P2PSand.
 443 By construction, the influence of the DEM global damping parameter becomes
 444 more significant when the regime commences being far from being quasi-static,
 445 which is expected to occur during such a dynamic event and the present section
 446 investigates in detail this influence for the present multi-scale simulations.

447 A numerical simulation is performed for the loose soil column by using dif-
 448 ferent DEM global damping coefficient values of 0.2 and 0 instead of the value
 449 of 0.6 that was employed during the previous simulations in Section 5.1 and the
 450 results are shown in Fig 24 and Fig 25. The simulation results demonstrate how
 451 the damping parameter affects the response at different levels of the column,
 452 whereby for the case of a damping value of 0.2 the top, middle and bottom
 453 zones final axial strain values increase by approximately 100%.

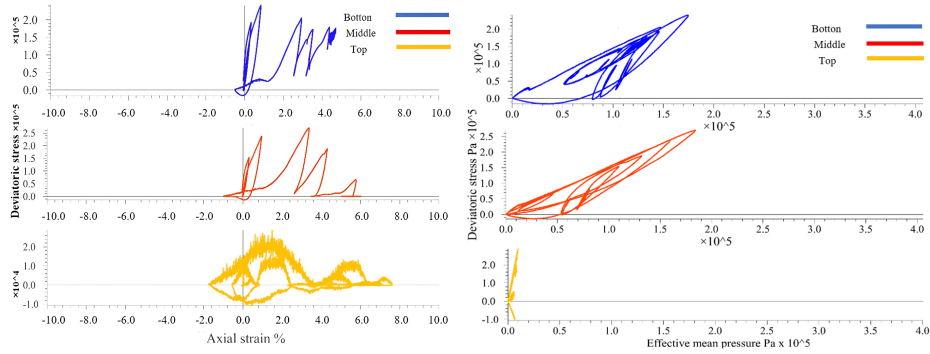


Figure 24: Multi-scale model predictions for a loose soil column $D_r = 25\%$ using global damping coefficient = 0.2.

454 Fig 25 also compares the effective mean pressure values for the three damping
 455 values at the end of the seismic event. Obviously, the damping parameter affects
 456 the distribution of the effective mean pressure and therefore, the liquefied zones
 457 throughout the soil column.

458 It is instructive at this point to study the effect of particle sizes in the DEM
 459 model (REV) during such dynamic events. The investigation is performed by
 460 using the two models in Fig. 6 in which only the particle size is changed while

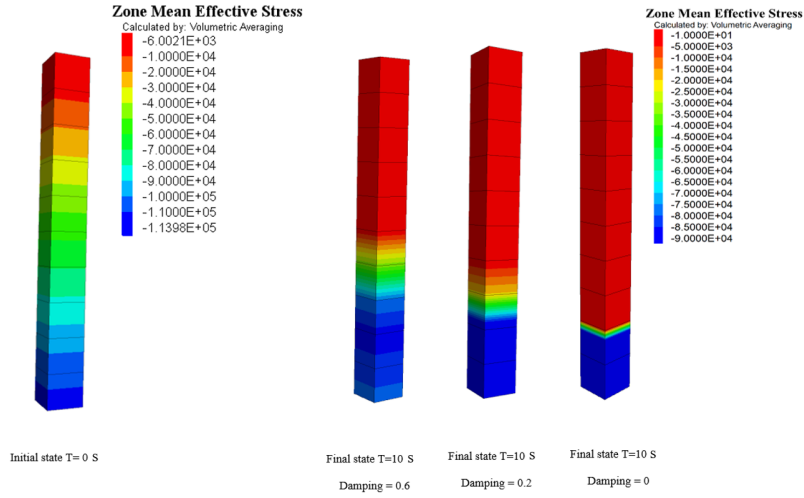


Figure 25: Initial and final values of the effective mean pressure (in Pa) through the column for different damping values for the loose case.

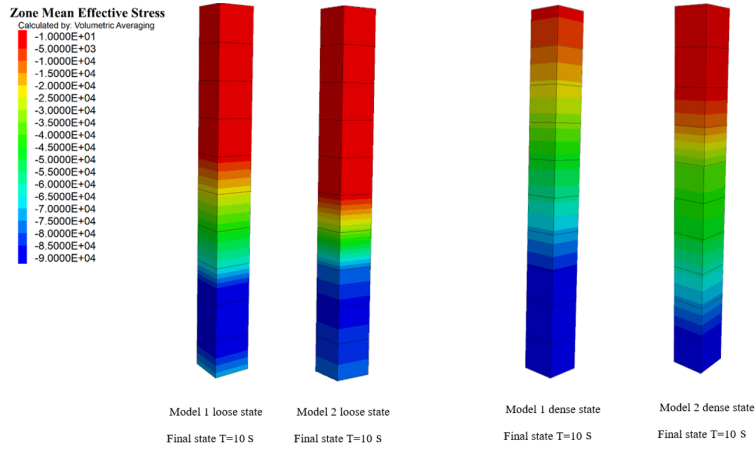


Figure 26: The final values of the effective mean pressure (in Pa) through the soil column for different particle size distributions for the loose (leftmost) and the dense (rightmost) cases and two different size distributions (gravel-like model 1 and sand-like model 2).

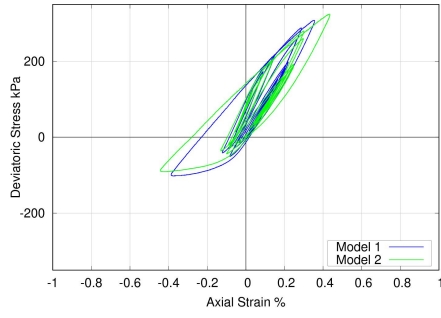
461 maintaining the same contact model, particle number, and damping coefficient.
462 The particle size distribution of model 1 could represent a gravel-filled soil col-
463 umn. The results in Fig. 26 show an influence of the particle size on the dis-
464 tribution of the effective mean pressure along the column, indicating that soils
465 with larger particles have less liquefaction potential due to their inertial effect.
466 As a matter of fact, a smaller grain size (or a lower inertial number from a
467 collisional I in the order of 10^{-2} to values around 10^{-3} , see later Fig. 29) leads
468 to an increase in reached strains as shown in Fig. 27 and Fig. 28, consistently
469 to previous Section 3.5.

470 The inertial number is evaluated to examine the dynamic effect on the pre-
471 vious simulations. Fig. 29 illustrates the evolution of the inertial number of the
472 top and the bottom zones for the loose case with a damping value = 0.6. For
473 model 1 the values of the inertial number indicate some dynamic effect on the
474 behavior of the top zone and bottom zone coherently with the previous discus-
475 sion in Section 3.5. Whereas the results of model 2 show only an intermittent
476 dynamic effect for the top zone at different stages during the event, which can be
477 attributed to lower effective mean pressure values and higher strain rate due to
478 the occurrence of the liquefaction. Thus, we recall that one of the main advan-
479 tages of DEM over constitutive models is its ability to consider the real physics
480 of granular materials by taking particle inertia into account during dynamic
481 simulations.

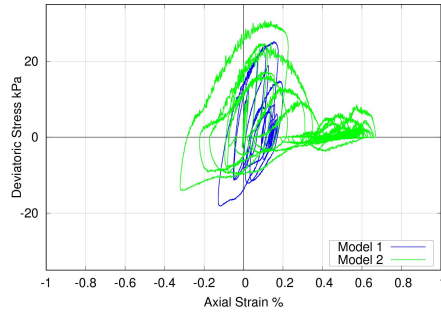
482 These inertial effects would combine in reality with another advantage of
483 gravel-like soils against sand soils through their higher hydraulic conductivity
484 “permeability” leading to dissipate faster pore pressure (which is not computed
485 in the present simulation).

486 *5.3. Discussion about the advantages and limitations of P2PSand and spherical* 487 *DEM-based multiscale approaches*

488 From the multi-scale model results in Fig. 16 and Fig. 17, it can be deduced
489 that when an unloading path is imposed after a dilatation behavior (evolu-
490 tion on the failure envelope in an undrained condition), more plastic defor-
491 mation and pore pressure are generated resulting in a significant decrease in

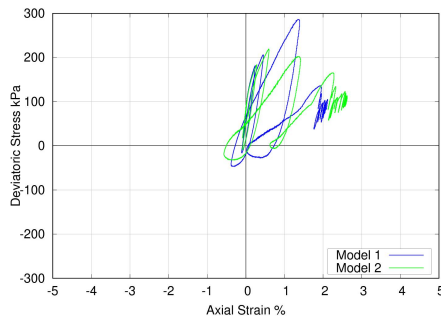


(a) Bottom zone $D_r = 60\%$

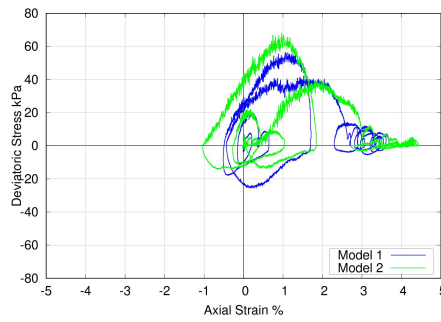


(b) Top zone $D_r = 60\%$

Figure 27: Effect of particle size on the response of the dense soil column for the bottom and top zones with a damping value = 0.6.



(a) Bottom zone $D_r = 25\%$



(b) Top zone $D_r = 25\%$

Figure 28: Effect of particle size of the response on the loose soil column for the bottom and top zones with a damping value = 0.6.

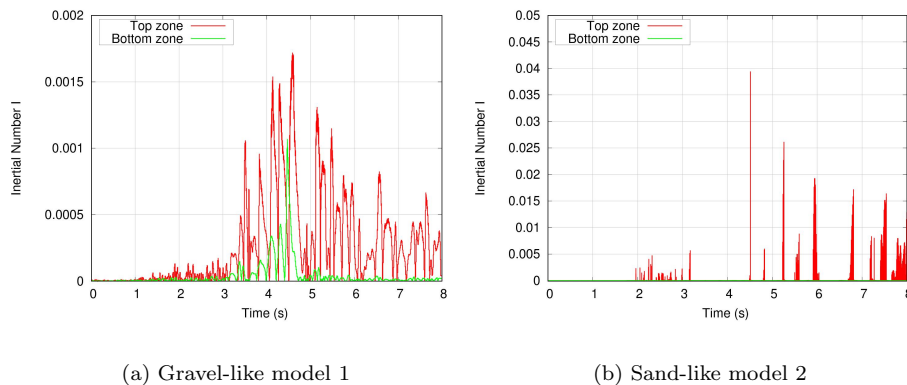


Figure 29: The evolution of the inertial number for the bottom and top zones in the case of damping = 0.6 for $D_r = 25\%$ and different particle sizes.

492 effective mean pressure and deviatoric stress. However, despite the fact that
 493 the P2PSand model incorporates the influence of fabric evolution (noting that
 494 fabric anisotropy develops only when the dilatancy occurs) on the dilatancy be-
 495 havior, the results of the P2PSand model contradict the DEM results at this
 496 point (which is more pronounced for the dense state, see $q - p'$ curves in Fig.
 497 16 and Fig. 17). These results recommend calibrating the fabric parameters
 498 of the P2PSand model on cyclic triaxial for dense samples with dilative be-
 499 havior. Also, they suggest to revisit the P2PSand model formulation for the
 500 stiffness-dilatancy degradation law.

501 On the other hand, the multi-scale approach provided an adequate seismic
 502 response by using four contact parameters (which could be reduced to three
 503 parameters in the case of a more realistic particle shape, as illustrated by Mo-
 504 hamed et al. (2022)) and excluded all nonphysical responses that occurred when
 505 constitutive models were used, as previously discussed. However, difficulties
 506 still remain when attempting to reproduce high-precision qualitative results for
 507 cyclic triaxial undrained tests as shown previously in Section 3.3 due to switch-
 508 ing between triaxial compression and triaxial extension at each cycle, which
 509 can be attributed to the use of spherical particles and the lack of initial fab-
 510 ric consideration. Also, as highlighted by Mohamed et al. (2022) (Figs. 18-19

511 therein), although the spherical shapes together with the rolling resistance con-
 512 tact model can provide a good agreement with the experimental triaxial tests,
 513 irregular shapes still better match the experimental data in terms of the initial
 514 slope in the $q - \epsilon_a$ curve, volumetric contraction behavior and stress softening
 515 behavior.

516 One should additionally consider the small strain properties of soil (Hardin
 517 and Richart Jr, 1963; Tatsuoka et al., 1979), i.e. the small-strain modulus G_{max}
 518 because of its important role in wave propagation mechanisms and liquefaction
 519 potential. Fig. 30 shows the prediction of the DEM model for the relation
 520 $G_{max} - p'$ estimated from undrained triaxial tests at 10^{-5} strain amplitude
 521 together with experimental data by Tatsuoka et al. (1979). While the DEM
 522 results are of the correct order of magnitude, with just a 26% discrepancy for
 523 the smallest confining pressures considered in the study (50 kPa), they also
 524 confirm that the linear rolling resistance contact model used in this study in
 525 conjunction with spherical particles cannot offer the expected mean pressure
 526 dependency of small-strain modulus G_{max} on the effective mean pressure p' (as
 527 adopted in the P2PSand model in Eq. A.5). Therefore, a more adequate contact
 528 formulation could improve the DEM REV behavior in this aspect, such as the
 529 Hertz model (Itasca, 2018; Mindlin and Deresiewicz, 1953) or a more advanced
 530 contact model as adopted by Kuhn (2022).

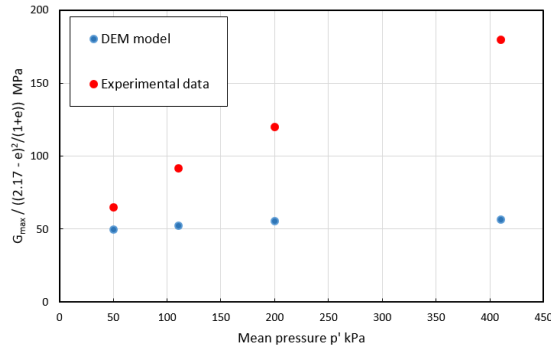


Figure 30: Comparison between the DEM model (initial void ratio = 0.63) and experimental data from Tatsuoka et al. (1979) for the relationship between small-strain modulus G_{max} and mean pressure p' for Toyoura sand.

531 As another important issue, the spherical model has a strong tendency to
 532 show isotropy (as it is the case after the isotropic preparation phase, Table 2),
 533 lacking inherent fabric anisotropy which would induce for instance anisotropic
 534 elastic characteristics and possibly impact seismic waves propagation.

535 Finally, Table 3 summarizes the different modeling choices for the multi-
 536 scale and DEM models and highlights the achievements and shortcomings of
 537 the proposed approach.

Table 3: Commented summary of the different modelling choices within the multi-scale and DEM models.

Modelling topic	Chosen approach	Remark
Proposed multi-scale approach		
Coupling Scheme	FVM-DEM FLAC3D-PFC	No need for a tangent stiffness matrix Less computational time
Stress matrix expression	Inclusion of inertial effects in DEM	Appropriate for seismic and dynamic simulations
Hydro-mechanical coupling	Inclusion of mechanically-induced pore pressure evolution	Darcy's law not activated herein
Used DEM model		
Particles shape	Spherical	10 - 100 times faster computational time (Mohamed et al., 2022; Duriez and Bonelli, 2021)
Contact model	Rolling resistance model with constant stiffness	Not able to reproduce $G_{max} - p'$ curve
Packing and its preparation	Isotropic packing with 7000 particles	Appropriate REV is achieved Lack of inherent anisotropy
Calibration and validation at lab-scale	Calibration on monotonic and cyclic tests while using same void ratio as experiments	Very good prediction for monotonic loading Less precise prediction for cyclic tests

538 5.4. Computational time and software parallelization aspects

539 In terms of computational time, executing the FLAC3D-PFC multi-scale
 540 model is logically significantly longer than a pure FLAC3D simulation: 6 hours
 541 vs 20 minutes for the current study respectively, as obtained utilizing a worksta-
 542 tion with 8 cores, 3.0 GHz CPU and 64 GB RAM. Since differences in operations
 543 reduce to the application of the DEM or P2PSand models as a constitutive rela-
 544 tion, it is evident that the majority of the time cost for the multi-scale coupling
 545 comes from PFC-DEM computations. The amount of the latter is directly

546 proportional to the number of zones, with evident higher costs to be expected
547 for more complex BVP in terms of mesh than the one considered here. On
548 the other hand, the present choice of studying a 1D wave propagation is not
549 computationally important in itself and 2D or 3D propagation studies with a
550 similar number of zones, if possible, would show the same time requirements.

551 In order to alleviate DEM-induced time costs, one should note that PFC
552 supports parallel DEM simulations by distributing the computational load on
553 the available cores allowing multi-threaded computation for contact detection
554 and contact model with an efficient spatial searching and contact detection
555 scheme.

556 It could also be thought of to apply parallelization to FLAC3D structure-
557 scale operations with simultaneous computations of DEM REVs, as discussed
558 e.g. by Kuhn (2022).

559 **6. Concluding summary and perspectives**

560 This paper compares a discrete-based approach and one advanced bound-
561 ing surface plasticity model 'P2PSand' for sand behavior and the propagation
562 of seismic waves after a fair calibration and validation procedure of the two
563 approaches on lab experiments. A 3D multi-scale FVM \times DEM scheme is es-
564 tablished between a continuum code Flac3D and discrete element PFC code to
565 solve boundary value problems by using the DEM as a constitutive model.

566 Thanks to its use of the common and well-documented FLAC3D-PFC codes,
567 as well as the ingredients of the coupling scheme (e.g., inertial effect), the pro-
568 posed model can be used within various complex 3D numerical simulations for
569 soils, including cyclic and shock loading. Also, the implementation of the present
570 multi-scale scheme is less complex than the FEM \times DEM scheme found in the
571 literature since in the explicit FVM \times DEM scheme there is no need to establish
572 a consistent tangent stiffness matrix from the macroscopic computation, which
573 can reduce the computational time of simulations. Numerical results demon-
574 strate the accuracy of the implemented coupling scheme through classical stress
575 paths applied on one or two zones. On the other hand, proper implementation

576 and application of the averaged stress tensor calculated from the DEM part
577 require careful treatment. The inertial term in the homogenization formula of
578 stress for granular assembly is shown to be an essential term during dynamic
579 simulations with higher inertial number values, such as severe earthquakes and
580 impact loadings. It is found that by increasing the inertial number, the strength
581 of the granular material increases, accompanied by more dilative behavior and
582 no clear critical state condition.

583 The DEM and P2PSand models have been calibrated and validated based on
584 experimental laboratory data of Toyoura sand for monotonic and cyclic loadings.
585 The validated DEM model is used via multi-scale modeling to analyze the wave
586 propagation mechanism in a saturated soil column made of Toyoura sand and
587 is compared with the predictions of the P2PSand model. Results reveal several
588 differences in response evolution logic between the two models. First, the so-
589 called butterfly loops in the effective stress plane and the hysteretic loops in the
590 deviatoric axial strain plane are quite different for the two models under dense
591 and loose cases. Second, for dense and loose conditions, the P2PSand model
592 accumulates more axial strain than the multi-scale model, resulting in a possible
593 underestimation of the resistance of any earth structure under cyclic loadings.

594 In addition, the parametric study performed on the effect of the DEM nu-
595 merical damping coefficient highlighted the importance of this parameter during
596 seismic or dynamic events. Results of the propagation of seismic waves show
597 that different damping values can affect the final distribution of pore pressure
598 as well as the final deformation of the column. In such a case, minimizing the
599 DEM global damping parameter is essential to ensure more realistic results and
600 avoid an artificial decrease in strain estimations that would be detrimental to
601 structural stability in engineering studies. As for the particle size effect, it is
602 found that the two models with different particle size distributions are influ-
603 enced by some dynamic effect in different ways. First, for the model that has
604 the same size as Toyoura sand, the behavior was quasi-static during the first
605 stage of the event, however, when liquefaction occurred at some positions in
606 the soil column, the behavior became more dynamic due to the low value of the

607 effective mean pressure. As for the case with larger particle size, the simulations
608 are shown to be dynamic by tracking the values of the inertial number which
609 indicates that soils with larger particles have a greater dynamic contribution to
610 stress that leads to less liquefaction potential.

611 Finally, the computational time for the multi-scale model is significantly
612 longer, taking six hours compared to a 20-minute simulation in the case of the
613 P2PSand model. However, considering the precision of the multi-scale method,
614 this computational time is quite acceptable.

615 Further perspective for this work is to investigate cyclic behavior and multi-
616 scale modeling of the behavior of the polyhedron DEM model also presented
617 in (Mohamed et al., 2022) since the latter is more realistic, e.g., for what con-
618 cerns initial fabric consideration (material inherent anisotropy) than the present
619 spherical model. First, to verify to what extent the initial fabric consideration
620 could improve the cyclic behavior and cyclic mobility of a DEM model compared
621 to experimental data. Second, to quantify its influence on the final values of
622 strain and effective mean pressure for boundary value problems, e.g., comparison
623 between the polyhedron and sphere DEM models for the previous example of
624 seismic wave propagation. In addition, we intend to use the present multi-scale
625 scheme for modeling the seismic behavior of a real earth dam.

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635 **Appendix A. P2PSand Constitutive formulas**

636 A power relationship relating here the critical relative density D_{rc} to p'
 637 across different ranges of the confining pressures:

$$D_{rc} = D_{rc0} + \lambda_c \left(\frac{p'}{p_{atm}} \right)^\zeta \quad (\text{A.1})$$

638 Where λ_c , ζ and D_{rc0} are three positive model parameters.

$$I_p = \frac{p'}{p_c} \quad (\text{A.2})$$

639 Eq. (A.1) is complemented in the (deviatoric) stress space by a critical state
 640 surface giving the $M = \sqrt{3/2} \|\mathbf{s}\|/p$ ratio at the critical state, M^c for any Lode
 641 angle θ , from its critical values during triaxial compression and triaxial exten-
 642 sion. Denoting the latters M_{comp} and M_{ext} respectively and $c = M_{ext}/M_{comp}$
 643 the corresponding ratio as a model parameter, the same Lode angle dependency
 644 than Cheng and Detournay (2021) is considered:

$$\frac{M^c(\theta)}{M_{comp}} = g(\theta, c) = \left(\frac{2c^4}{c^4 + 1 + (c^4 - 1) \cos 3\theta} \right)^{0.25} \quad (\text{A.3})$$

645 The critical-strength parameter M_{comp} may be expressed in the form of a
 646 Mohr-Coulomb friction angle for the same triaxial compression path, ϕ_{comp} .

647 At the other end of the behavior, for small deformations, the incremental
 648 form of the elastic part is defined as follows:

$$dp' = -K d\epsilon_v^e \quad d\mathbf{s} = 2G d\mathbf{e}^e \quad (\text{A.4})$$

649 Where p' is the effective mean stress (isotropic stress) and \mathbf{s} is the deviatoric
 650 stress tensor. K and G are bulk and shear modulus respectively. ϵ_v and \mathbf{e} are
 651 volumetric strain and deviatoric strain tensor respectively. The P2PSand hypo-
 652 elastic law is adopted for expressing K and G as a function of the current relative
 653 density and the current mean effective pressure :

$$G = G_0 (D_r + C_{Dr}) p_{atm} \left(\frac{p'}{p_{atm}} \right)^n \quad K = \frac{2(1 + \nu)}{3(1 - 2\nu)} G \quad (\text{A.5})$$

654 The model proposes a power law for the bounding and dilatancy surfaces.
655 The form of these surfaces is the same as the critical state surface and has an
656 additional dependency on the relative state index I_p and relative density D_r as
657 follows:

$$M^d(\theta) = M^c(\theta)I_p^{(n_d D_r)} \quad M^b(\theta) = M^c(\theta)I_p^{(-n_b D_r)} \quad (\text{A.6})$$

658 where $M^d(\theta)$ and $M^b(\theta)$ denote dilatancy and bounding surfaces respectively.
659 Finally, the images of the kinematic hardening tensor $\boldsymbol{\alpha}$ on the dilatancy and
660 bounding surfaces are defined as the intersection points between a parallel line
661 to the loading direction \mathbf{n} stemming from the origin point to the dilatancy or
662 bounding surfaces as shown in Fig. 1. \mathbf{n} is the loading direction tensor outward
663 along the radius $\mathbf{r} - \boldsymbol{\alpha}$ and is defined as:

$$\mathbf{n} = \frac{\mathbf{s} - p'\boldsymbol{\alpha}}{\|\mathbf{s} - p'\boldsymbol{\alpha}\|} \quad (\text{A.7})$$

664 The image tensors on the different surfaces can be expressed as follows:

$$\boldsymbol{\alpha}_\theta^{d,b,c} = \sqrt{2/3}[g(\theta, c)M^{d,b,c} - m]\mathbf{n} \quad (\text{A.8})$$

665 The plastic volumetric strain can be related to dilatancy as follows:

$$d\epsilon_v^p = \langle L \rangle D \quad (\text{A.9})$$

666 For virgin loading, the dilatancy is defined based on the distance between the
667 current $\boldsymbol{\alpha}$ and its image on the dilatancy surface $\boldsymbol{\alpha}_\theta^d$ as proposed by Dafalias
668 and Manzari (2004).

$$D = A_d(\boldsymbol{\alpha}_\theta^d - \boldsymbol{\alpha}) : \mathbf{n} \quad (\text{A.10})$$

669 where A_d is a model variable that depends on the fabric state and will be
670 defined later. If the state of $\boldsymbol{\alpha}$ is inside the MBS, a new term will be added to
671 the dilatancy equation to avoid the overshooting of the dilatancy during cyclic
672 loading as follows:

$$D_{Cyc} = A_{d0}(\boldsymbol{\alpha}_\theta^d - \boldsymbol{\alpha}) : \mathbf{n} * k_{Cyc}(\boldsymbol{\alpha} - \boldsymbol{\alpha}_{in}) : \mathbf{n} \quad (\text{A.11})$$

673 where k_{cyc} is a calibration parameter for cyclic loading. In the present model
 674 fabric tensor dz evolution is described as follows:

$$dz = - \langle L \rangle c_z (\sqrt{\frac{2}{3}} z_{max} \mathbf{n} + z), D > 0 \quad (\text{A.12})$$

675 The fabric tensor z evolves only during dilatancy dilation. Finally, dilatancy
 676 is impacted by the fabric evolution as follows:

$$A_d = A_{d0} (1 + \sqrt{\frac{2}{3}} \langle z : \mathbf{n} \rangle) \quad (\text{A.13})$$

677 Appendix B. Flac3D continuum equations

678 The momentum principle of motion (Cauchy's equations) is:

$$\sigma_{ij,j} + \rho b_i = \rho \frac{dv_i}{dt} \quad (\text{B.1})$$

679 For a body in equilibrium or steady state Eq. B.1 is reduced to :

$$\sigma_{ij,j} + \rho b_i = 0 \quad (\text{B.2})$$

680 In Flac3D, the equation of motion is applied to the mesh nodes. To this end,
 681 the finite volume approximation of the space derivative is applied to obtain a
 682 description of the strain rate tensor as a function of nodal velocities by assuming
 683 that the velocity field varies linearly inside the tetrahedron. The Gauss diver-
 684 gence theorem to the tetrahedron relates the divergence of the velocity field
 685 inside a volume V and the flux through a surface S as follows:

$$\int_V v_{i,j} dV = \int_S v_i n_j dS \quad (\text{B.3})$$

686 where $v_{i,j}$ is the gradient of the velocity field and n_j is the normal to the surface.
 687 The infinitesimal strain rate tensor is defined as:

$$\epsilon_{ij} = \frac{1}{2} (v_{i,j} + v_{j,i}) \quad (\text{B.4})$$

688 The average velocity of each face of tetrahedron $\bar{v}_i^{(f)}$ can be defined from their
 689 nodal velocities as follows :

$$\bar{v}_i^{(f)} = \frac{1}{3} \sum_{l=1, l \neq f}^4 v_i^l \quad (\text{B.5})$$

690 where the superscript l represents the nodal number. From Eq. B.3, the strain
 691 rate tensor in Eq. B.4 and Eq. B.5 can easily define the relation between strain
 692 rate tensor and nodal velocities.

$$\epsilon_{ij} = \frac{1}{6V} \sum_{l=1}^4 \left(v_i^l n_j^{(l)} + v_j^l n_i^{(l)} \right) S^{(l)} \quad (\text{B.6})$$

693 The final goal is to apply the equation of motion to the different nodes by
 694 using an explicit finite difference approximation to the time derivative. In order
 695 to obtain the nodal formulation of the equation of motion, the concept of virtual
 696 work is applied to a tetrahedron by multiplying the net force in Eq. B.1 by an
 697 imaginary velocity applied at the tetrahedron centroid as follows:

$$\delta P = (\sigma_{ij,j} + \rho b_i - \rho \frac{dv_i}{dt}) \cdot \delta v_i = 0 \quad (\text{B.7})$$

698 where P is the power. Since the velocity varies linearly inside the tetrahedron,
 699 dv_i can be expressed as a function of nodal velocity as follows:

$$\delta v_i = \frac{1}{4} \sum_{n=1}^4 \delta v_i^n \quad (\text{B.8})$$

700 The internal power can be expressed as a function of nodal velocities and the
 701 nodal force vector T_i^l (from Cauchy's formula) as follows:

$$T_i^l = \sigma_{ij} n_j^{(l)} S^{(l)} \quad (\text{B.9})$$

702

$$P^{Internal} = -\frac{1}{3} \sum_{l=1}^4 \delta v_i^l T_i^l \quad (\text{B.10})$$

703 In turn, the external power done by the body force and inertial force is expressed
 704 as follows:

$$P^{External} = \sum_{n=1}^4 \delta v_i^n \left[\frac{\rho b_i V}{4} - \frac{\rho V}{4} \left(\frac{dv_i}{dt} \right)^l \right] \quad (\text{B.11})$$

705 where $\frac{\rho V}{4}$ is the nodal mass m^l . From Eq. B.11 and Eq. B.10, the nodal
 706 formulation of the equation of motion can be expressed as:

$$m^l \left(\frac{dv_i}{dt} \right)^l = \frac{T_i^l}{3} + m^l b_i + P_i^l = F_i^l \quad (\text{B.12})$$

707 where F_i^l is the out-of-balance force and P_i^l is the external force applied to
 708 a node. Finally, the explicit finite difference approximation for the derivative
 709 $(\frac{dv_i}{dt})^l$ to obtain the new nodal velocity is as follows:

$$v_i^{<l>}(t + \frac{\Delta t}{2}) = v_i^{<l>}(t - \frac{\Delta t}{2}) + \frac{\Delta t}{m^{<l>}} F_i^{<l>} \quad (\text{B.13})$$

710 The present multi-scale model also includes hydro-mechanical coupling as avail-
 711 able in FLAC3D with, for the present saturated conditions:

$$\boldsymbol{\sigma}' = \boldsymbol{\sigma} - p\mathbf{I} \quad (\text{B.14})$$

$$\frac{1}{M} \frac{\partial p}{\partial t} = -q_{i,i} + q_v - \alpha_{Biot} \frac{\partial \epsilon}{\partial t} \quad (\text{B.15})$$

712 Where $\boldsymbol{\sigma}'$ is effective stress and \mathbf{I} is the Kronecker tensor. $\frac{\partial p}{\partial t}$ is the variation of
 713 pore pressure with respect to the time, M is the Biot modulus ($= k_f$ here), α_{Biot}
 714 is the Biot coefficient ($= 1$ here) and ϵ is the mechanical volumetric strain. q_i is
 715 the specific discharge vector described by Darcy's law $q_i = -k_i \nabla p$ (k_i and ∇p are
 716 mobility coefficients matrix and pressure head gradient) and q_v is the volumetric
 717 fluid source intensity respectively. These last two terms are disregarded here
 718 even though they could be included by activating fluid flow option in FLAC3D.

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