

1 **Numerical DEM analysis of small-strain stiffness under anisotropic stress**
2 **states**

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7 **Abstract.**

8 This contribution assesses the influence of stress anisotropy on stiffness using discrete
9 element method (DEM) simulations of true-triaxial tests supplemented with analytical
10 studies. The samples considered comprised normally consolidated random
11 monodisperse samples. The simulations were carried out at four different mean stress
12 levels; at each stress level various combinations of the three principal stresses were
13 considered. Stiffness was measured using planar wave propagation simulations. Using
14 regression analysis it is shown that density effects can be considered using void ratio
15 correction factors derived for isotropically compressed samples. However, a void ratio
16 correction factor that considers coordination number is seen to be more marginally
17 appropriate than the conventional form used in geotechnical experimental work.
18 Material exponents that quantify the influence of each stress component on the stiffness
19 were then determined. Analytical expressions derived from effective medium theory are
20 less effective than the correction functions following the form used in current
21 experimental practice.

22 **Keywords:** small-strain stiffness, stress anisotropy, true-triaxial tests.

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23 Introduction

24 The power-law relationship between elastic shear stiffness and mean effective stress,
25 $G_0 \propto p'^n$ is well established (Hardin & Richart 1963; Houlsby & Wroth 1991). The
26 relative magnitudes of the principal stress components also impact the stiffness values.
27 Bellotti et al. (1996) experimentally related stiffness to all three principal stresses using
28 the following expression (modified from the original form):

$$G_0 = C_p F(e) (\sigma_{prop})^{n_{prop}} (\sigma_{osc})^{n_{osc}} (\sigma_{third})^{n_{third}} \quad (1)$$

29 where $F(e)$ is a normalizing function to eliminate void ratio effects, and C_p is a
30 (dimensional) experimentally determined material constant. The stresses in the
31 directions of propagation and oscillation of the stress wave are denoted σ_{prop} and σ_{osc} ,
32 respectively, while the remaining orthogonal stress is denoted σ_{third} ; typically these
33 stresses correspond to the principal stresses. The material exponents n_{prop} , n_{osc} and
34 n_{third} quantify the influence of each principal stress on G_0 .

35 Referring to prior studies of stiffness using discrete element method (DEM) (e.g. Khalili
36 et al. 2017; Magnanimo et al. 2008), where particle-scale data are available a more
37 appropriate form of Equation 1 might be:

$$G_0 = F(e, C_N, \chi, \nu_p, E_p) (\sigma_{prop})^{n_{prop}} (\sigma_{osc})^{n_{osc}} (\sigma_{third})^{n_{third}} \quad (2)$$

38 where C_N is the average coordination number, χ is a measure of the orientation fabric
39 and ν_p and E_p are the Poisson's ratio and Young's modulus of the solid particle material,
40 and the units of $F(e, C_N, \chi, \nu_p, E_p)$ must ensure dimensional consistency.

41 Most prior research has concurred that only σ_{prop} and σ_{osc} measurably influence the
42 elastic stiffness (e.g. Roesler 1979). O'Donovan et al. (2015) used DEM simulation data
43 considering lattice packings and a limited number of stress combinations to argue that
44 σ_{third} also has finite influence on G_0 . These limitations compromised the clarity of their
45 data and consequently the generality of their conclusions. This contribution addresses
46 the resultant gap in understanding by using an improved DEM simulation approach to
47 assess the material behaviour over a range of p' values and a large number of
48 permutations/combinations of the three principal stresses in each case. The shear
49 stiffnesses were determined using wave propagation, reflecting the popularity of bender
50 element testing in experimental soil mechanics research. Dynamic bender element

51 testing is attractive as is difficult to measure stiffnesses at very small strains accurately
52 using conventional, load-deformation techniques even where local deformation
53 transducers are mounted to measure locally (Clayton, 2011); furthermore when used in
54 a triaxial cell bender elements can give the shear moduli in the principal stress planes
55 (Lings et al. , 2000) and they can be mounted in a wide range of apparatuses (Clayton,
56 2011; Hamlin, 2014). The DEM wave propagation simulations were supplemented with
57 and stress probes.

58 **DEM simulation approach**

59 The simulation approach broadly follows that documented in Otsubo et al. (2017) and
60 Nguyen et al. (2017). For completeness, a brief overview is provided here. A modified
61 version of the granular LAMMPS code was used (Plimpton, 1995), with a simplified
62 Hertz-Mindlin contact model; simulation parameters are summarized in Table 1. Rigid
63 wall boundaries were applied perpendicular to the direction of wave propagation while
64 the remaining lateral boundaries were periodic to minimize boundary effects (Figure 1).

65

66 Random monodisperse dense and loose samples (RMD and RML respectively) were used.
67 The randomly packed specimens were created from an initial cloud of 34986 non-
68 contacting particles; a two-stage compression process was used. The dense random
69 samples (RMD) were initially isotropically compressed to a mean effective stress, p' , of
70 1 kPa with $\mu_p = 0$ while $\mu_p = 0.15$ for the first compression stage for the loose samples
71 (RML). The interparticle friction was then increased to $\mu_p = 0.35$. After modifying μ_p ,
72 there was a subsequent servo-controlled isotropic compression to a target confining
73 pressure of $p' = 70$ kPa, $p' = 200$ kPa, $p' = 700$ kPa, or $p' = 7000$ kPa (depending
74 on the final p' required). Then starting from each of these isotropic stress states, the
75 principal stresses were either maintained constant or increased to generate various
76 combinations of stress anisotropy with target values of $p' = 100$ kPa, $p' = 300$ kPa,
77 $p' = 1000$ kPa, or $p' = 10000$ kPa. Using this approach each sample was then isotropic
78 and normally consolidated; there was inherent anisotropy induced by previous loading
79 or by simulation of a deposition process. The stress combinations were constrained so
80 that the minimum and maximum principal stresses considered were $\sigma_3 = 0.75p'$ and
81 $\sigma_1 = 1.25p'$ respectively, to avoid gross yield. These stress combinations are similar to
82 those that are considered in physical cubical cell experiments (e.g. Hamlin, 2014)

83

84 Figure 2(a) illustrates the variation in C_N , with the geometric mean of the stresses in
85 oscillation and propagation directions ($\sqrt{\sigma_{osc}\sigma_{prop}}$) for each simulation considered,
86 while Figure 2(b) illustrates the variation in the average mechanical coordination
87 number, C_N^* , (calculated by excluding particles with 0 or 1 contacts) with $\sqrt{\sigma_{osc}\sigma_{prop}}$.
88 Both sets of data indicate that, at a given value of p' , there is not a significant variation
89 in the number of contacts in the sample as a function of the stress anisotropy; nor are
90 there significant variations in void ratio (Figure 2(c)). Note that the relationship between
91 void ratio and coordination number is not unique; Magnanimo et al. (2008) who also
92 considered monodisperse samples, applied a particular DEM simulation approach which
93 achieved random dense samples with C_N value that varied between 4.88 and 6.65 all with
94 a void ratio ≈ 0.64 .

95

96 Once the desired stress state was achieved, shear waves were generated by applying a
97 single-period sine motion to one rigid wall and the change in stress measured at the
98 opposite wall was used to determine the shear wave velocity (V_s) using the peak-peak
99 method as described in Otsubo et al. (2017) and Nguyen et al. (2017). To avoid inter-
100 particle sliding, following Magnanimo et al. (2008) during stress wave propagation, $\mu_p =$
101 0.45 was used for both RMD and RML samples. The corresponding shear modulus was
102 then calculated as $G_0^{DEM} = \rho V_s^2$ where ρ is the sample density ($\rho = \frac{\rho_p}{1+e}$, ρ_p is the particle
103 density). At each p' value 14 to 16 simulations were performed for each sample type.

104

105 To confirm that the wave propagation simulations give reasonable stiffness values, small
106 stress increment triaxial probes were simulated. In these probes the vertical stress was
107 increased by $\delta\sigma_z = 1$ kPa while the horizontal stresses were maintained constant ($\delta\sigma_x =$
108 $\delta\sigma_y = 0$) to obtain the equivalent stiffness, $G_{equ}^{prob} = \delta q / 3\delta\varepsilon_s$ ($\delta q = \delta\sigma_z - \delta\sigma_x$) and the
109 shear strain increment is $\delta\varepsilon_s = 2(\delta\varepsilon_z - \delta\varepsilon_x) / 3$; $\delta\varepsilon_z$ and $\delta\varepsilon_x$ are the principal strain
110 increments in z and x directions respectively). For a real soil with an anisotropic fabric
111 this stiffness value does not correspond to either G_{zx} or G_{zy} (e.g. Lings et al. 2011).
112 However for the isotropic random samples here there should be agreement; for the
113 random dense sample with $p' = 300$ kPa, $G_{equ}^{prob} = 279.3$ MPa, $G_{zx}^{DEM} = 280.9$ MPa and

114 $G_{zy}^{DEM} = 281.6$ MPa; confirming the ability of the dynamic simulations to give a correct
115 measure of stiffness. Note that one could also use the analytical approach proposed by
116 Agnolin and Roux, (2007) to determine the stiffness tensor from the particle-scale data
117 available from the DEM simulations.

118

119

120 **Simulation results**

121 Previous empirical investigations (Hardin & Blandford 1989; Sadek et al. 2007) assumed
122 $n_{prop} = n_{osc}$ and neglected the contribution of σ_{third} ; consequently correlations of the
123 form $G_{oscprop} \propto (\sigma_{osc}\sigma_{prop})^n$ were explored as in Figure 3. The data for the random
124 samples give $n = 0.355$ for RMD samples and $n = 0.388$ for RML samples; these are
125 close to the exponent $n = 0.333$ that is obtained by applying effective medium theory
126 (EMT) to a random packing of spherical particles for this Hertzian contact model (Walton,
127 1987; Chang et al., 1991; Liao et al., 2000) .

128 For the three sample types considered, the exponent, n , observed for the scenario where
129 p' remains constant differs from the n value that fits the data when p' varies. In all three
130 cases the relationship between G_0 and $\sigma_{osc}\sigma_{prop}$ depends on the stress anisotropy. The
131 n values (obtained from least squares regression) for the isotropic stress cases are
132 measurably higher than n values obtained by fitting a line to the data obtained for the
133 various stress combinations examined at a given p' value. In comparison with the RMD
134 samples, there is more scatter in the data for the RML sample.

135 Here ν_p and E_p are constant for all the simulations and so, to facilitate examination of the
136 G_0 dependancy on σ_{prop} and σ_{osc} , referring to Equation 2, an appropriate function
137 $F^*(e, C_N, \chi)$ was sought so that the influence of stress could be appropriately isolated.

138 To remove the influence of stress and fabric anisotropy equivalent simulations on
139 isotropic samples with the same particle parameters documented in Otsubo (2016) were
140 considered. Referring to Figure 4, 7 DEM samples were created and the friction coefficient
141 was varied so that the void ratio at 1kPa ranged from 0.545 to 0.689. Each of these
142 samples was then isotropically compressed to 10 MPa and G_0 values were determined
143 systematically during the compression. Following earlier soil mechanics research

144 (Hardin and Richart 1963), assuming such correction function, considering void ratio
145 alone takes the form $F(e) = \frac{(B-e)^2}{1+e}$ and, applying regression analysis to the entire dataset
146 gives a value of $B = 1.186$ (Otsubo 2016). Referring to Figure 5(a) when the $\frac{G_0}{F(e)}$ data are
147 considered a clearer correlation with $\sqrt{\sigma_{osc}\sigma_{prop}}$ emerges, and the differences between
148 loose and dense and isotropic and anisotropic stress states are less apparent. Revisiting
149 the data on Figure 4, B appears to be stress-level dependent and a simple curve fitting
150 gives $B^p = \exp(-0.1 + 0.046p')$; use of this approach effectively unifies the loose and
151 dense data (Figure 5(b)); however both the correction and the stiffness now have a
152 stress- dependency. One can also isolate particles that contributed to the stress
153 transmission network and consider only particles with at least two contacts, so that $e^* =$
154 $\frac{V_{Total} - \sum_{i=2}^{\infty} V_s^i}{\sum_{i=2}^{\infty} V_s^i}$ in which V_s^i is the sum of the volume of particles with a coordination
155 number i , and V_{Total} is the total sample volume. Using e^* and again assuming a functional
156 form $F(e^*) = \frac{(B^* - e^*)^2}{1 + e^*}$, gives $B^* = 1.484$; application of this correction factor is less effective
157 at unifying the data than the pressure-sensitive correction (Figure 5(c)).

158
159 To assess the relative merits of these void ratio corrections linear regression analyses
160 were applied to Equation 1, where the unknown parameters are C_p , n_{prop} , n_{osc} , and
161 n_{third} . These regressions are compared with the DEM data on Figures 6(a) and (c); while
162 the resulting exponent values are provided on Table 2.

163
164 Effective medium theory (EMT) indicates that for an isotropic stress state a correction
165 factor of the form $F^{EMT}(e, C_N) = [C_N/(1 + e)]^{2/3}$ can be used. The results support an idea
166 that the normalized stiffness ($G/(F(e^*))$) has a power-law dependency on C_N ; i.e.

$$F(e, C_N) = \frac{(B^* - e^*)^2}{1 + e^*} C_N^\alpha \quad (3)$$

167 Figure 6 (b) gives the resulting regression; and includes comparison of a regression
168 including only $F(e^*)$. Comparing values of the ratio of the prediction of the regression
169 and the simulation data are plotted as a function of $\sqrt{\sigma_{osc}\sigma_{prop}}$ on Figure 6(c) and (d);
170 confirming that including C_N improves the prediction, but that the discrepancy can be as
171 large as 5.6%. Referring to the summary of the relative errors on Table 3, there are minor
172 improvements in the predictive ability of the regression when comparing the case with

173 $B = 1.186$ and e with the other correction options considered. It is important to
174 recognize however that the dataset does not include samples at the same void ratio with
175 differing coordination numbers.

176

177 Excluding the case where B is varied with p' , whichever correction function is applied the
178 contributions of n_{prop} and n_{osc} greatly exceed the contribution of n_{third} however it is
179 difficult to clearly say whether σ_{prop} or σ_{osc} dominates.

180

181 The correction function $F(e)$ is clearly empirical and based on experimental practice.
182 Informed by EMT, Figure 7 considers the data from an alternative perspective. EMT
183 suggests a correlation between G_0 and $[C_N/(1 + e)]^{2/3}$ and this is confirmed in Figure
184 7(a) (neglecting consideration of the stress anisotropy G_0 is normalized by $E_p^{2/3} p'^{1/3}$).
185 For the relatively small stress anisotropies considered here a clear trend emerges; these
186 data indicate a dependency of G_0 on both the C_N and e in line with EMT. However the
187 data on Figure 7(b) show that normalization of the G_0 data by the product $E_p^{2/3} p'^{1/3} \times$
188 $[C_N/(1 + e)]^{2/3}$ is less effective than use of the $F(e) = \frac{(B-e)^2}{1+e}$ or its variants considered
189 above; these observations also hold for the isotropic dataset developed by Otsubo (2016).
190 Yimsiri and Soga (2000) attributed the inability of EMT to capture the stress-dependancy
191 of soil stiffness to its inability to capture variations in fabric with stress. In their DEM
192 simulations, Magnanimo et al (2008) found that the variation of $G_0 / p'^{1/3}$ with C_N
193 differs from the EMT prediction. More sophisticated theoretical EMT expressions
194 (e.g. Thornton, 1993) also failed to capture the observations noted here;
195 assumptions such as affine deformations and irrotational particles limit use of this
196 theory.

197

198 Referring to Figure 8(a) there is a clear link between the stiffness ratio and the stress
199 ratio; as would be expected from Equation 1. Inclusion of various measures of fabric
200 anisotropy in the regression analyses did not support further extension of the correction
201 function to include a χ term. This can be understood by reference to Figure 8(b); for
202 these samples with only stress induced anisotropy the fabric and stress anisotropies are
203 closely linked and so the χ term cannot be considered an independent variable.

204

205

206 **Conclusions**

207 DEM simulations of dynamic plane wave propagation have been used to consider the
208 influence of stress anisotropy on sample stiffness in a fundamental manner and the
209 following observations are made.

210 1. In the absence of a void ratio correction relationships between stiffness and the
211 principal stresses (i.e. between G_0 and $\sqrt{\sigma_{osc}\sigma_{prop}}$) differ for the cases of isotropic
212 compression, where p' is varied, and anisotropic compression, at a constant p' .

213 2. Application of void ratio functions derived using equivalent samples subject to
214 isotropic stress states unifies the dense and loose sample at each stress level for all the
215 stress anisotropies considered and confirms the negligible influence of σ_{third} .

216 3. The empirical void ratio correction function with a form $F(e) = \frac{(B-e)^2}{1+e}$ served better to
217 unify the data than a normalization derived from isotropic EMT which has already been
218 shown to have limited validity.

219 4. Regression analysis that incorporates the $F(e^*)$ correction function and assumes a
220 power-law correlation with the coordination number give a only slightly better match to
221 the simulation data when compared with a macro-scale, conventional void ratio
222 correction function. However these conclusions may not be universally applicable; the
223 C_N - e relationship is not unique, and this data set does not include samples with similar
224 void ratios and very different coordination numbers as were examined by Magnanimo et
225 al. (2008).

226 5. For the samples considered here the stress and fabric anisotropies are closely linked
227 and so inclusion of a fabric term, independent of stress, in the overall expression for
228 stiffness cannot be justified.

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234

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