

1           **ON THE INTERNAL STRUCTURE QUANTIFICATION FOR GRANULAR**  
2                           **CONSTITUTIVE MODELLING**

3                           **Xia Li<sup>a\*</sup>**

4   <sup>a</sup> Department of Chemical and Environmental Engineering, Faculty of Engineering, University Park,  
5   The University of Nottingham, Nottingham, NG7 2RD, UK

6   **ABSTRACT**

7           The importance of internal structure on the stress-strain behavior of granular materials has  
8   been widely recognized. How to define the fabric tensor and to use it in constitutive modelling  
9   however remains an open question. The definition of fabric tensor requires 1) identifying the  
10   key aspects of structure information and 2) quantifying their impact on material strength and  
11   deformation. This paper addresses these issues by applying the homogenisation theory to  
12   interpret the multi-scale data obtained from the discrete element simulations. Numerical  
13   experiments have been carried out to test granular materials with different particle friction  
14   coefficients. More frictional particles tend to form less but larger void cells, leading to a larger  
15   sample void ratio. Upon shearing, they form more significant structure anisotropy and support  
16   higher force anisotropy, resulting in higher friction angle. Material strength and deformation  
17   have been explored on the local scale with the particle packing described by the void cell system.  
18   Three groups of fabric tensor have been covered in this paper. The first one is based on the  
19   contact vectors, which is the geometrical link between contact forces and material stress. And  
20   their relationship with material strength has been quantified by the Stress-Force-Fabric  
21   relationship. The second group is based on as the statistics of individual void cell characteristics.  
22   Material dilatancy has been interpreted by tracing the void cell statistics during shearing. The

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\* Corresponding author. Address: Department of Chemical and Environmental Engineering, Faculty of Engineering, University Park, University of Nottingham, Nottingham, NG7 2RD, United Kingdom, Email: xia.li@nottingham.ac.uk. Tel: +44(0)1159514167. Fax: +44(0)1159513898.

23 last group is based on the void vectors, for their direct presence in the micro-structural strain  
24 definition, including those based on the void vector probability density and mean void vector.

25 Correlations among various fabric quantifications have been explored. The mean void  
26 vector length and the mean void cell area are parameters quantifying the internal structure size,  
27 and strongly correlated with each other. Anisotropy indices defined based on contact normal  
28 density, void vector density, void vector length and void cell orientation are found effective in  
29 characterizing loading-induced anisotropy. They are also closely correlated. In-depth  
30 investigation on structural topology may help establish the correlation among different fabric  
31 descriptors and unify the fabric tensor definition. Deformation bands have been observed to  
32 continuously form, develop and disappear over a length scale of several tens of particle  
33 diameters. Its relation to and impact on material deformation is an area of future investigation.

34 **Keywords:** Fabric quantification, Granular statistics, Homogenisation theory, Discrete  
35 Element Method (DEM).

## 36 INTRODUCTION

37 Different from metal, the complexity in the stress-strain behaviour of granular materials is  
38 largely rooted in the packing formation and evolution upon shearing. It is widely acknowledged  
39 that the fabric tensor needs to be introduced into constitutive modelling to capture the main  
40 features of granular material behaviour. A number of fabric definitions have been proposed  
41 (Satake 1982, Oda 1985, Li and Li 2009, Nguyen, Magoaric et al. 2009, Kruyt and Rothenburg  
42 2014). Generally speaking, the appropriateness of fabric definition depends on its application.  
43 Targeting at constitutive modelling, this paper interprets the material strength and deformation  
44 from the local scale in order to shed some light on the important and yet to answer questions,  
45 including 1) what is the most appropriate fabric definition used for modelling the material  
46 stress-strain behaviour and 2) how to effectively incorporate it to reflect the impact of internal

47 structure on the material stress-strain responses.

48 Among many interesting earlier discoveries, (Satake 1978)'s graph-theoretical approach  
49 is instrumental in establishing the correspondence between discrete and continuum  
50 representations and informing the advancement of homogenisation theory. (Satake 1983)  
51 replaced an assembly of grains with graphs and formulated the mathematical expressions of  
52 discrete granular mechanics. The importance of voids has been recognized and emphasized by  
53 introducing dual particles to represent void spaces. In line of Satake's pioneering work, (Bagi  
54 1996) introduced the concepts of two dual cell systems as the geometric representation of  
55 discrete assemblies, and building upon it, the duality of the stress and strain. (Li and Li 2009)  
56 extended the concept to three dimensional spaces by modifying the Voronoi-Delaunay  
57 tessellation systems with consideration of whether the particles are in real contact or not. In two  
58 dimensional spaces, their dual cell systems are equivalent to Satake's dual graphs. Interestingly,  
59 the idea of describing the material internal structure with a tessellation system has also been  
60 developed, though separately, in the field of granular statistics by (Blumenfeld and Edwards  
61 2006). Instead of using two dual systems, they represent the granular structure with a set of  
62 grain polygons and void polygons.

63 With the internal structure described by the dual graphs or its analogues, the continuum  
64 scale stress tensor has been expressed in terms of particle interactions and contact vectors which  
65 are geometrical quantities in the solid cell system connecting contact points and particle centres.  
66 This correspondence has been theoretically established on Newton's second law of motion  
67 (Christoffersen 1981, Rothenburg and Selvadurai 1981, Bagi 1996, Kruyt and Rothenburg 1996,  
68 Li, Yu et al. 2009). In parallel, the continuum-scale strain tensor has been expressed in terms  
69 of particle relative displacements and geometrical quantities in the void cell systems based on  
70 the compatibility condition (Bagi 1996, Kruyt and Rothenburg 1996, Kuhn 1999, Li, Yu et al.  
71 2009). The importance of internal structure is self-evident with the presence of local

72 geometrical quantities in these two discrete expressions.

73       These theoretical developments in the homogenization theory have also laid down the  
74 groundwork to systematically investigate how the internal structure impacts on the stress-strain  
75 behavior from the local scale. In this study, numerical experiments have been carried out using  
76 the Discrete Element Method (DEM) (Cundall and Strack 1979) to provide the multi-scale data.  
77 A series of numerical simulations have been carried out on granular assemblies with identical  
78 particle geometries but different friction coefficients. The void cell system has been constructed  
79 to describe particle packing, and the continuum-scale material behavior is considered as the  
80 collective response from all individual void cells. Discussions have been extended to the  
81 definition of fabric tensor, which serves as a necessary state variable in constitutive modelling  
82 (Li and Dafalias 2012).

### 83 **NUMERICAL SIMULATIONS**

84       Numerical experiments have been carried out using the commercial package, Particle Flow  
85 Code (PFC2D), a two dimensional Discrete Element Method (DEM) software (Itasca  
86 Consulting Group Inc. 1999). The boundary control algorithm introduced in (Li, Yu et al. 2013)  
87 has been used to impose the target loading path. The particles are circular disks uniformly  
88 distributed in number within the range of (0.1mm, 0.3mm). The thickness of particles is set as  
89 0.2 mm. The particle interactions are of linear stiffness with a slider. The normal and tangential  
90 stiffnesses are set as  $1.0 \times 10^5$  N/m. A series of simulations have been carried out with the particle  
91 friction coefficient  $\mu_p$  being 0.0, 0.1, 0.2, 0.5, 1.0 and 10.0 respectively. The specimens are  
92 hexagonal except for the case of  $\mu_p = 10.0$ , when the contact sliding is nearly prohibited,  
93 extremely large contact forces have been observed around the corner indicating local strong  
94 arching formation. The dodecagonal sample shape is hence used. The boundary properties are  
95 set as the same as the particle properties.

96

97

Figure 1 Void ratio prior to shearing vs particle friction coefficient

98

99 The samples are prepared using the deposition method. Particles are generated in a  
100 rectangular region whose height is twice the width. The particles deposit vertically at gravity  
101  $G = 100\text{m/s}^2$  in the low damping environment to form the initial packing, which is then  
102 trimmed by the prescribed boundary and consolidated to  $p_c = 1000\text{kPa}$  for shearing. The scaled  
103 gravity is used to reduce computational time. Such prepared samples are expected to be initially  
104 anisotropic, although as shown later, of limited magnitude. For the series of numerical  
105 experiments carried out in this study, the numbers of particles range from 3,443 to 3,938  
106 depending on the particle friction coefficient. The ratio between the sample size and the particle  
107 diameter is around 60, and is believed to be large enough to serve as representative elements.  
108 Due to the difference in particle friction coefficients, different initial structures are formed. Fig.  
109 1 plots the void ratio of the samples, an index of packing density, at their initial (pre-shearing)  
110 states, which is observed to increase with the increase in particle friction coefficient. The  
111 packing with  $\mu_p = 10.0$  has a similar void ratio to the packing with  $\mu_p = 1.0$ . This  
112 information is not included in the figure for better illustration of the variation when the friction  
113 coefficient varies between 0 and 1.

114 In analogy to drained tests, samples are sheared in the vertical direction while the mean  
115 normal pressures  $p = (\sigma_1 + \sigma_2)/2$  are kept constant. The boundary control algorithm detailed  
116 in (Li, Yu et al. 2013) has been used to control the displacements of boundary walls  
117 synchronously to impose the strain-controlled boundary, and to monitor the stress boundary  
118 using a servo-controlled mechanism. Local damping has been used to dissipate excess kinetic  
119 energy during shearing. Loading increments are only imposed when both the equilibrium  
120 criteria and the specimen boundary conditions are satisfactorily met. The material responses are

121 shown in Fig. 2 by plotting the stress ratio  $\eta = q / p = 2(\sigma_1 - \sigma_2) / (\sigma_1 + \sigma_2)$  and the volumetric  
122 strain  $\varepsilon_v$  against the deviatoric strain  $\varepsilon_q$ , where  $\sigma_1$  and  $\sigma_2$  are the major and minor principal  
123 stresses respectively in two dimensional spaces. The stress ratio is related to material frictional  
124 angle as  $\eta = 2 \sin \phi$ .

125

126 Figure 2 Material responses to shearing (a) Stress ratio b) Void ratio

127

128 The deposition method is expected to produce loose specimens. Most of the samples show  
129 strain hardening behavior however strain softening response has been observed in samples with  
130 high particle friction coefficients  $\mu_p = 1.0$  and  $\mu_p = 10.0$ . The friction angles are observed to  
131 be low in general because circular particles have been used in the simulations. Similar to the  
132 observations in (Peyneau and Roux 2008), the sample made of frictionless particles ( $\mu_p = 0.0$ )  
133 exhibits a low shear resistance and little volume change. It flows nearly as a fluid, with the  
134 sample friction angle as low as  $4.6^\circ$ . A very low and fluctuating volumetric strain up to 0.2% is  
135 observed. The sample frictional angle increases gradually to  $14^\circ$  when the particle friction  
136 coefficient increases to 0.2. However, further increase in particle friction coefficient doesn't  
137 further increase the material shear resistance. This is consistent with the laboratory (Skinner  
138 1969) and numerical (Thornton 2000, Antony and Sultan 2007, Huang, Hanley et al. 2014)  
139 observations on 3D granular materials. The volume change exhibits more diversity. When the  
140 particle friction coefficient increases from 0 to 0.2, the sample becomes more contractive with  
141 the volumetric strain with  $\mu_p = 0.2$  going up to 1%. However, when the particle friction  
142 coefficient increases further to  $\mu_p = 0.5$ , the sample contracts slightly and then behaves dilative.  
143 Further increase in particle friction coefficient leads to more dilative behavior with the  
144 volumetric strain with  $\mu_p = 10.0$  as high as 2.8%. It is also observed that although the variation

145 in stress ratio occurs mainly in the first 10% deviatoric strain, the change in volumetric strain  
146 continues until much larger strain levels.

## 147 **FABRIC QUANTIFICATION PERTINENT TO MATERIAL SHEAR RESISTANCE**

148 The external loading is transmitted throughout the specimen via the force-bearing structure.  
149 Fig. 3 plots the force chains at the initial states. The heterogeneity in particle interaction is clear  
150 from the figure. It is observed that strong forces appear periodically over every few particle  
151 diameters. Since the chosen sample size is much larger than the dimension exhibited in force  
152 heterogeneity, the samples are considered as representative elements for stress analyses.  
153 Comparing Fig.3(a) & (b), samples of higher particle friction coefficients exhibit a periodicity  
154 over a slightly larger length scale.

155

156 Figure 3 Contact force distribution prior to shearing (a)  $\mu_g = 0.0$  and (b)  $\mu_g = 1.0$ . (The  
157 thickness of the black lines is proportional to the magnitude of contact forces)

158

## 159 **The Stress-Force-Fabric Relationship**

160 Granular materials are known for its ability to self-organize their internal structure.  
161 Anisotropy develops as a result of shearing and makes an important contribution to material  
162 shear resistance. This section addresses the fabric quantification pertinent to the shear resistance  
163 of granular material in aid of the Stress-Force-Fabric relationship, which was originally  
164 proposed by (Rothenburg and Bathurst 1989). It was established based on the micro-structural  
165 definition of stress tensor, linking the continuum scale stress tensor  $\sigma_{ij}$  with contact forces

166  $f_i^c$  and contact vectors  $v_i^c$  as:

$$167 \quad \sigma_{ij} = \frac{1}{V} \sum_{c \in V} v_i^c f_j^c \quad (1)$$

168 in which  $V$  stands for the volume of interest. Note that a contact point is identified only when  
 169 there is non-zero interaction between two entities. At an internal contact point between two  
 170 particles, there is always a pair of action and reaction forces corresponding to two contact  
 171 vectors pointing from the contact point to each particle centre. They are counted as two contacts.  
 172 However, an external contact point between particle and boundary wall is only counted once.

173 (Li and Yu 2013) employed the theory of directional statistics (Kanatani 1984) to  
 174 investigate the statistics of particle-scale information, characterised the directional dependence  
 175 of particle-scale information with direction tensors and formulated the Stress-Force-Fabric  
 176 relationship in the tensorial form. The notations used in (Li and Yu 2013, Li and Yu 2014) are  
 177 followed in this paper. Examination of the particle-scale statistics supports the following  
 178 simplifications:

- 179 1) There is a slight and isotropic statistical dependence between contact forces and  
 180 contact vectors which can be approximated by  $\langle v_i f_j \rangle_{\mathbf{n}} = \zeta \langle v_i \rangle_{\mathbf{n}} \langle f_j \rangle_{\mathbf{n}}$  where  $\zeta$   
 181 is a scalar around 1.025 for all the simulations. In this expression,  $*|_{\mathbf{n}}$  denotes the  
 182 value of variable  $*$  in direction  $\mathbf{n}$ , and  $\langle * \rangle_{\mathbf{n}}$  denotes the average value of all terms of  
 183  $*$  sharing the same direction  $\mathbf{n}$ ;
- 184 2) The contact vector length is isotropic;
- 185 3) The contact normal probability density can be sufficiently accurately approximated by  
 186 up to the 2<sup>nd</sup> rank polynomial series of unit directional vector  $\mathbf{n}$ ;
- 187 4) The mean contact force  $\langle \mathbf{f} \rangle_{\mathbf{n}}$  can be sufficiently accurately approximated by up to the  
 188 3<sup>rd</sup> rank polynomial series of unit directional vector  $\mathbf{n}$ .

189 Eq. (1) can be converted into integration over direction by grouping the terms with the same  
 190 contact normal directions together. Combined with the above observations, the simplified  
 191 Stress-Force-Fabric relationship can be written as:



192 
$$\sigma_{ij} = \frac{\omega^p N^p}{2V} \zeta v_0 f_0 \left[ (1+h) \delta_{ij} + G_{ji}^f + \frac{1}{2} D_{ij}^c + G_{ij}^v \right] \quad (2)$$

193 where  $\omega^p$  is the particle coordination number,  $N^p$  is the number of particles,  $v_0$  is the  
 194 directional average of mean contact vector and  $f_0$  is the directional average of mean contact  
 195 force,  $h$  is a scalar accounting for the contribution from the joint products which increases  
 196 slightly from 0 to around 0.01 during shearing. In two dimensional spaces, the direction tensor  
 197 for contact normal density is  $D_{ij}^c = d^c \begin{pmatrix} \cos \phi^c & \sin \phi^c \\ \sin \phi^c & -\cos \phi^c \end{pmatrix}$ , where  $d^c$  denotes the magnitude  
 198 of directional variation and  $\phi^c / 2$  indicates the preferred principal direction of contact normal  
 199 density.  $G_{ij}^f = B^f \begin{pmatrix} \cos \beta^f & \sin \beta^f \\ \sin \beta^f & -\cos \beta^f \end{pmatrix}$  is the 2<sup>nd</sup> rank tensor characterizing the directional  
 200 dependence of contact forces, where  $B^f$  denotes the magnitudes of directional variation,  $\beta^f$   
 201 indicates its preferable principal direction. It is worth pointing that  $G_{ij}^f$  covers the contributions  
 202 from both the normal contact force components and the tangential contact force components.  
 203  $G_{ij}^c$  is defined similar to  $G_{ij}^f$  but characterises the statistics of contact vectors.

204 Approximation using Eq. (2) has been found to give exact matches of the continuum-scale  
 205 stress, and provides a valid point to interpret material strength from the particle scale.

## 206 **Fabric quantification**

207 The micro-structural stress definition given in Eq. (1) shows that the particle-scale  
 208 geometrical information linked to the material stress is contact vectors. And the SFF  
 209 relationship given as Eq. (2) provides the analytical relationship quantifying the correlation  
 210 between the contact vectors and material stress state. Considering the different nature in the  
 211 normal and tangential force-displacement relationship, the terms in Eq. (1) has been grouped  
 212 based on their contact normal directions, and the deviatoric tensor  $D_{ij}^c$  in Eq. (2) reflects the

213 anisotropy in contact normal density. The anisotropy in contact vector is a secondary factor  
 214 which can be characterized in terms of  $G_{ij}^c$ . These two aspects can be combined and quantified  
 215 in terms of one fabric tensor. This section summarises their definitions and calculations based  
 216 on directional statistical theories.

217 *Fabric quantification for contact normal density*

218 Contact normal based fabric tensor is one of the most widely used index in characterizing  
 219 the loading induced anisotropy (Oda, Nemat-Nasser et al. 1985), and appears in Eq. (2) as

220 
$$D_{ij}^c = d^c \begin{pmatrix} \cos \phi^c & \sin \phi^c \\ \sin \phi^c & -\cos \phi^c \end{pmatrix},$$
 which is called the fabric tensor of the third kind (Kanatani 1984).

221 It describes the variation of contact normal density over direction. An equivalent definition is  
 222 the fabric tensor of the second kind  $F_{ij}^c$  (Kanatani 1984). With them, the contact normal density  
 223 distribution can be approximated as:

224 
$$E^c(\mathbf{n}) = \frac{1}{E_0} F_{ij}^c n_i n_j = \frac{1}{E_0} (1 + D_{ij}^c n_i n_j) \quad (3)$$

225 where  $E_0 = \oint_{\Omega} d\Omega = 2\pi$  in the two dimensional spaces.  $D_{ij}^c$  and  $F_{ij}^c$  are interchangeable as

226 
$$F_{ij}^c = D_{ij}^c + \delta_{ij} \quad (4)$$

227 They can be determined from the fabric tensor of the first kind, also referred to the moment

228 tensor  $N_{ij}^c$  in (Kanatani 1984, Li and Yu 2013) as  $F_{ij}^c = 4 \left( N_{ij}^c - \frac{1}{4} \delta_{ij} \right)$  and  $D_{ij}^c = 4 \left( N_{ij}^c - \frac{1}{2} \delta_{ij} \right)$ ,

229 where the moment tensor can be calculated as:

230 
$$N_{ij}^c = \langle n_i n_j \rangle = \frac{1}{M} \sum_{\alpha=1}^M n_i^{\alpha} n_j^{\alpha} \quad (5)$$

231 where  $\mathbf{n}^{(1)}, \mathbf{n}^{(2)}, \dots$  and  $\mathbf{n}^{(N)}$  being the unit vectors representing contact normals.  $M$  is the  
 232 total number of contacts.

233 *Fabric quantification for contact vector anisotropies*

234 The anisotropy in mean contact vector could be an additional contributor to material stress  
 235 ratio as listed in the Stress-Force-Fabric relationship, Eq. (2), for non-spherical particles (Li and  
 236 Yu 2014), although its anisotropy magnitude is often found to be secondary compared with that  
 237 of contact normal density. The mean contact vector  $\langle v_j \rangle|_n$  can be approximated as  
 238  $\langle v_j \rangle|_n = v_0 (n_j + G_{ji}^c n_i)$ , or equivalently in terms of the fabric tensor  $H_{ij}^c = v_0 (1 + G_{ij}^c)$ , where  $v_0$   
 239 is the directional average of mean contact vector.

240 *Fabric quantification combining contact normal and contact vector anisotropies*

241 A combined account for the contribution of material fabric to stress state may include both  
 242 contact normal density and contact vector anisotropy, and be defined on the contact vector  
 243 based moment tensor as:

$$244 \quad L_{ij}^c = \langle v_i n_j \rangle = \frac{1}{M} \sum_{\alpha=1}^M v_i^\alpha n_j^\alpha \approx \oint_{\Omega} E^c(\mathbf{n}) \langle v_i \rangle|_n n_j d\Omega \quad (6)$$

245 Substituting Eq. (3) into Eq.(6) leads to  $L_{ij}^c = v_0 \left[ \frac{1}{2} (\delta_{ij} + G_{ij}^c) + \frac{1}{4} (D_{ij}^c + D_{im_1}^c G_{jm_1}^c) \right]$  in 2D spaces.

246 Note  $D_{ij}^c$  and  $G_{ij}^c$  are deviatoric tensors. Neglecting the joint products of higher rank terms for

247 simplicity and denoting the normalized deviator tensor as  $C_{ij}^c = \frac{2L_{ij}^c}{L_{kk}^c} - \delta_{ij} = G_{ij}^c + D_{ij}^c / 2$ , the

248 Stress-Force-Fabric relationship can be rewritten as:

$$249 \quad \sigma_{ij} = \frac{\omega^p N^p}{2V} \varsigma v_0 f_0 (\delta_{ij} + C_{ij}^c + G_{ji}^f) \quad (7)$$

250 where  $L_{ii}^c = v_0$ .  $C_{ij}^c$  provides an explicit account of the impact of internal structure on material  
 251 strength.

252 **The micromechanical interpretation of material shear resistance**

253 In this study, disk-shaped particles are used. The mean contact vector has been found

254 nearly isotropic so that  $G_{ij}^c=0$  and  $C_{ij}^c = D_{ij}^c/2$ . For all the simulations, the principal fabric  
255 directions are the same as the loading direction, and the material anisotropy can be characterized  
256 in terms of the degrees of contact normal anisotropy  $d^c$ , which is plotted in Fig. 4(a). Even for  
257 frictionless particles, shearing results in structure anisotropy, although of limited magnitude.  
258 More significant fabric anisotropy develops in more frictional particles. Upon shearing, the  
259 contact normal anisotropy increases mostly monotonically, although in more frictional samples,  
260 its rate of increases is observed to be higher and reaches a stronger anisotropy at the critical  
261 state. When the friction coefficient increases further beyond  $\mu_p = 0.5$ , the evolutions of contact  
262 normal anisotropy are observed to no longer change. This is similar to the observation made in  
263 (Huang, Hanley et al. 2014) based on 3D DEM simulations.

264

265 Figure 4 The micro-mechanical contributors to material strength (a) Contact normal  
266 anisotropy  $d^c$ , and (b) Contact force anisotropy  $B^f$

267

268 Information on contact force anisotropy  $B^f$  is plotted in Fig. 4(b). While particle friction  
269 coefficient increases, both the contact normal anisotropy and the contact force anisotropy  
270 increase. The contact force anisotropy however exhibits a peak before approaching the critical  
271 state, coincident with the occurrences of peak stress ratio followed by strain softening. It is  
272 interesting to point out that no matter what the particle friction coefficient is, the anisotropy in  
273 contact force is of similar magnitude with contact normal anisotropy, which is better shown in  
274 Fig. 5 by plotting the two anisotropies against each other. The reference line indicates when the  
275 two anisotropic degrees are equal to each other. The strong correlation between the contact  
276 normal anisotropy and the contact force anisotropy is evident with most data points falling near  
277 the reference line. Shearing motivates contact force anisotropy slightly faster and higher than

278 the developed contact normal anisotropy. For samples made of very rough particles, contact  
279 force anisotropy was observed to be higher than the contact normal anisotropy at the early stage  
280 of shearing. When approaching the critical state, the two anisotropies become equal.

281

282 **Figure 5 Correlation between the fabric and contact force anisotropy**

283

284 In a summary, SFF relationship supports the effectiveness of  $D_{ij}^c$  and  $C_{ij}^c$  as the fabric  
285 tensor definition to study the material stress and hence strength. The force anisotropy is found  
286 strongly associated with the observed fabric anisotropy, in particular at the critical state. Hence,  
287 material shear strength can be determined from the fabric anisotropy should there be an  
288 established fabric-force correlation.

## 289 **VOID CELL STATISTICS AND MATERIAL DILATANCY**

290 In this section, the relationship between material dilatancy and the evolution of void cell  
291 statistics will be explored by viewing a granular assembly as a collection of void cells. The void  
292 cell system is formed by connecting contact points and particle centres. Particles without  
293 contribution to the global force transmission, including those with few than two contact points,  
294 are excluded during the void cell construction. The number of constitutive particles in void cells  
295 should be no less than 3. Fig. 6 provides an example by presenting the void cell system with  
296  $\mu_p = 0.5$ . The color scheme is associated with the void cell area. The void cells between  
297 boundary particles and walls have been identified in order to tessellate the whole space enclosed  
298 by the specimen boundaries.

299

300 **Figure 6 The void cell system at pre-shearing stage ( $\mu_p = 0.5$ )**

301

## 302 Void cell characterisation and void cell based fabric tensor

303 Viewing a granular material as an assembly of void cells, the material fabric tensor can be  
304 defined as the statistical average of individual void cell characteristics. The loop tensors used  
305 in (Nguyen, Magoariec et al. 2009, Kruyt and Rothenburg 2014) are such examples. However,  
306 there is no unique way in doing so. Here, the individual void cell is characterized based on the  
307 area moment of inertia, and the void cell based fabric tensor is proposed as their statistical  
308 average as one example of its kinds.

### 309 *Characterisation of individual void cells*

310 Void cells may have different and irregular shapes. A single dimension is inadequate to  
311 describe the geometry of individual void cells. Factors of primary interest are the size of the  
312 void cell, its shape and the orientation. The area moment of inertia  $I_{ij} = \oint_A r_i r_j dA$ , where  $r_i$  is  
313 the vector from the location of the area element  $dA$  to the area centre of void cell, contains all  
314 the necessary information and can be potentially used. Based on the area moment of inertia  $I_{ij}$ ,  
315 the tensor  $Z_{ij}$  is used to describe the local cell geometry:

$$316 \quad Z_{ij} = \frac{4}{A} I_{ij} \quad (8)$$

317 Its principle direction gives information on the void cell orientation.

318  
319 Figure 7  $\pi\sqrt{\det(Z_{ij})}$  vs. void cell area

320  
321  
322 In the case of an ellipse of semi-major axis of length  $a$  and semi-minor axis of length  $b$ ,

323  $Z_{ij} = \begin{pmatrix} a^2 & 0 \\ 0 & b^2 \end{pmatrix}$ . Note that the area of the ellipse is  $\pi ab = \pi\sqrt{J(\mathbf{Z})} = \pi\sqrt{\det(Z_{ij})}$ , where

324  $J(\mathbf{Z}) = \det(Z_{ij})$  denotes the Jacobian determinant of tensor  $Z_{ij}$ . This suggests that

325  $\pi\sqrt{\det(Z_{ij})}$  may serve as an effective estimation of void cell areas. Fig. 7 plots  $\pi\sqrt{\det(Z_{ij})}$   
326 against the area of void cells for all the void cells shown in Fig. 6. The red line in the figure  
327 plots the reference line  $y = x$ . Despite their irregular shape, the data have been found lying  
328 closely to, with most data slightly above, the reference line.

329 The shape of an ellipse can be described by the index  $(a-b)/(a+b)$ . For a circle, the  
330 index is equal to 0 and for an ellipse with infinite aspect ratio, it is 1. In terms of the tensor  
331 defined in Eq.(8), the equivalent expression is the void cell anisotropy index  
332  $\Delta^v = (\sqrt{Z_1/Z_2} - 1)/(\sqrt{Z_1/Z_2} + 1)$ , where  $Z_1$  and  $Z_2$  are the major and minor principal values  
333 of the fabric tensor  $Z_{ij}$ . Fig. 8 presents information on the shape of void cells by plotting the  
334 probability density function  $dP|_{\Delta^v \leq x}/d\Delta^v$ , where  $P|_{\Delta^v \leq x}$  represents the probability of void cells  
335 whose shape factor  $\Delta^v$  is no larger than  $x$ , and  $dP|_{\Delta^v \leq x}$  represents the probability of void cells  
336 whose shape factor falls within  $x - d\Delta^v/2 \leq \Delta^v = (\sqrt{Z_1/Z_2} - 1)/(\sqrt{Z_1/Z_2} + 1) \leq x + d\Delta^v/2$ . Fig.  
337 8(a) plots the probability density function at the initial state while Fig. 8(b) plots the probability  
338 density function after 20% deviatoric strain. It is observed that most void cells are anisotropic  
339 with the highest probability around  $\Delta^v = 0.2$ . For larger friction coefficients, the area fraction  
340 occupied by more anisotropic void cells becomes slightly larger while that by less anisotropic  
341 void cells becomes slightly smaller.

342

343 Figure 8 Probability Density Function  $dP|_{\Delta^v \leq x}/d\Delta^v$  (a) Deviatoric strain 0% (b) Deviatoric  
344 strain 20%

345

346 The fabric tensor for individual void cell  $S_{ij}^v$  is hence defined such that the major principal  
347 fabric as  $A^v(1 + \Delta^v)/2$ , the minor principal fabric as  $A^v(1 - \Delta^v)/2$  and the principal directions

348 are the same as those of  $Z_{ij}^v$ . Note that the ratio between the major and minor principal fabrics  
 349 is  $\sqrt{Z_1/Z_2}$ .

### 350 *Anisotropy in void cell orientation*

351 The orientation of void cells can be represented by a unit vector. Similar to contact normal  
 352 density, the void cell orientations can be characterised by the direction tensor with the form

$$353 \quad D_{ij}^S = d^S \begin{pmatrix} \cos \phi^S & \sin \phi^S \\ \sin \phi^S & -\cos \phi^S \end{pmatrix} \quad (9)$$

354 and calculated from its moment tensor, where  $d^S$  is the anisotropy index and  $\phi^S$  the principal  
 355 direction. The anisotropy index has been plotted in Fig. 9. The principal direction has been all  
 356 around  $90^\circ$ . The figure suggests that material anisotropy has developed as a result of more void  
 357 cells orienting towards the loading direction, similar to the observation reported in (Nguyen,  
 358 Magoaric et al. 2012).

359  
 360  
 361  
 362

Figure 9 Anisotropy in void cell orientations

### 363 *Void cell based fabric quantification*

364 The continuum-scale fabric tensor is defined as the average of void cell fabric tensors as:

$$365 \quad F_{ij}^S = \frac{1}{N^v} \sum_{v \in A} S_{ij}^v \quad (10)$$

366 The fabric tensors of individual void cells have been calculated from the void cell geometries  
 367 obtained from DEM simulations, and used to calculate the macro fabric tensor defined in Eq.

368 (10). The first invariant  $F_{ii}^S = \overline{A^v}$  is the average void cell area. The deviatoric part of  $F_{ij}^S$  is an  
 369 area-weighted measure of void cell shapes. The anisotropy index of void cell-based fabric  
 370 tensor, Eq.(10), is defined as  $d^F = 2(F_1^S - F_2^S) / (F_1^S + F_2^S)$ , where  $F_1^S$  and  $F_2^S$  are the



371 principal values of the fabric tensor  $F_{ij}^S$ . The principal direction is observed around  $90^\circ$ . Fig.  
 372 10 shows the evolution of the anisotropy index  $d^S$  during shearing, whose pattern is observed  
 373 in great similarity as that of contact normal density in Fig. 4(a) and that of void cell orientation  
 374 in Fig. 9, suggesting a strong correlation among these fabric indices, which will be explored  
 375 later in this paper.

376  
 377 Figure 10 Anisotropy index of  $F_{ij}^S$   
 378

### 379 **Material dilatancy and void cell statistics**

380 Dilatancy is the change in sample volume or void ratio during shearing. For 2D granular  
 381 assemblies, the total area of assembly  $A_{sam}$  is equal to the summation of all void cell areas and  
 382 can be expressed as:

$$383 \quad A_{sam} = \sum_{\alpha=1}^{N^v} A_v^\alpha = N^v \overline{A^v} \quad (11)$$

384 where  $A_v^\alpha$  denotes the area of the  $\alpha$ -th void cell,  $N^v$  the total number of void cells, and  $\overline{A^v}$   
 385 the average void cell area. The total particle (solid) area  $A_s = \sum_{\alpha=1}^{N^p} A_p^\alpha = N^p \overline{A^p}$ , where  $A_p^\alpha$   
 386 denotes the area of the  $\alpha$ -th particle,  $N^p$  is the total number of particles and  $\overline{A^p}$  is the average  
 387 particle area, a constant throughout the test. The void ratio of the granular assembly can hence  
 388 be formulated as:

$$389 \quad e = \frac{A_{sam}}{A_s} - 1 = \frac{N^v}{N^p} \frac{\overline{A^v}}{\overline{A^p}} - 1 \quad (12)$$

390 The total number of contacts can be found by summing up the coordination numbers of all  
 391 particles, which however may be slightly different from that summing over all the void cells  
 392 since in the void cell system each particle-wall contact is counted twice. Should the sample size  
 393 be large enough, the difference is small and negligible,  $M = N^p \omega^p = N^v \omega^v$ , where the void cell

394 coordination number  $\omega^v$  denotes the average number of constitutive particles in void cells. It  
 395 should be no less than 3 in two dimensional granulate systems. The material void ratio can  
 396 hence be rewritten as:

$$397 \quad e = \frac{\overline{A^v}}{\overline{A^p}} \frac{\omega^p}{\omega^v} - 1 \quad (13)$$

398 The volume change tendency, i.e., the dilatancy of granular material, can be quantified as the  
 399 change in the sample void ratio upon shearing, and studied by tracing the evolution of void cell  
 400 statistics, in particular  $\overline{A^v}/\overline{A^p}$  and  $\omega^v/\omega^p$  during shearing.

401 Fig. 11(a) plots the particle coordination number  $\omega^p$  and the void cell coordination  
 402 number  $\omega^v$  for pre-sheared samples with different particle friction coefficients. Fig. 11(b)  
 403 provides information of  $\overline{A^v}/\overline{A^p}$  and  $\omega^v/\omega^p$  at various friction coefficients. The data of  
 404  $\mu_p = 10.0$  are close to those of  $\mu_p = 1.0$ , and not shown in the figures. Note that the stability  
 405 condition of two dimensional infinite granulate system imposes the requirement of the minimal  
 406 coordination number being 3. The coordination numbers slightly smaller than 3 have been  
 407 observed in this study is partially because non-load bearing particles (rattlers) are present in the  
 408 system, but not excluded in particle coordination number. It is also because of the boundary  
 409 effect. At each boundary-particle contact point, there are two force components contributing to  
 410 the system stability. They are counted twice in void cell construction, but only once when  
 411 calculating the particle coordination number. For the same reasons, the relationship between  
 412 the particle coordination number  $\omega^p$  and the void cell coordination number  $\omega^v$  is found to  
 413 slightly deviate from the Euler's relation for planer graphs  $\omega^v = 2\omega^p / (\omega^p - 2)$  (Satake 1985).

414

415 Figure 11 The internal structure at initial states (a) Coordination number; (b) Void cell  
 416 characteristics

417

418 The figures show clearly that the particle friction coefficient has a significant effect on  
419 void cell characteristics. For frictionless particles, the particle coordination number is only  
420 slightly larger than that of void cells. The average void cell area and the average particle area  
421 are close. When the particles become frictional, the particle coordination number reduces while  
422 the void cell coordination number increases. More frictional particles tend to form fewer but  
423 larger void cells. It is observed that with increasing friction coefficients, the number of void  
424 cells drops, accompanied with an increase in void cell area. As a result, the average void cell  
425 area almost doubles when the particle friction changes from  $\mu_p=0$  to  $\mu_p=10$ . The increase in  
426 void cell area exceeds the reduction in void cell number, resulting in larger void ratios observed  
427 at higher friction coefficients.

428 The evolutions of the sample void ratio  $e$  and the void cell characteristics, including  
429  $\overline{A^v}/\overline{A^p}$ , the particle coordination number  $\omega^p$  and the void cell coordination number  $\omega^v$ , have  
430 been plotted in Fig. 12. Eq. (13) reveals that the change in the void ratio  $e$  is resulted from the  
431 competition between  $\overline{A^v}/\overline{A^p}$  and  $\omega^v/\omega^p$ . As seen in Fig. 12, when samples are sheared, the  
432 increase in void cell coordination number is observed and accompanied by an increase in the  
433 mean void cell area. When the increase in  $\overline{A^v}/\overline{A^p}$  exceeds that in  $\omega^v/\omega^p$ , the sample dilates  
434 with an increase in void ratio. Otherwise, the sample contracts with a reduced void ratio.

435 With zero and low particle frictions, the particle and void cell coordination numbers  
436 remain almost constant during shearing. However, for highly frictional particles, shearing  
437 causes significant reduction in particle coordination number and increase in void cell  
438 coordination number at the early stage of shearing, but this effect is overtaken by the increase  
439 in  $\overline{A^v}/\overline{A^p}$ . Samples show significant dilative responses. These changes during shearing are  
440 associated with the development of void cell anisotropies presented in Figs. 8, 9 & 10.

441

442 Figure 12 Evolution of void cell statistics to shearing (a) Void ratio  $e$ , (b)  $\overline{A^v}/\overline{A^p}$ , (c)

443 Particle coordination number  $\omega^p$  and (d) Void cell coordination number  $\omega^v$

444

#### 445 **The void cell coordination number**

446 Frictional particles tend to form larger void cells with higher coordination number.

447 Grouping the void cells according to their coordination number, the total sample area can be

448 expressed as:

$$449 \quad A_{sam} = \sum_{i=3} H|_{val=i} \overline{A^v}|_{val=i} = N^v \sum_{i=3} h|_{val=i} \overline{A^v}|_{val=i} \quad (14)$$

450 where  $H_{val=i}$  is the number of void cells whose coordination number is  $i$ ,  $h|_{val=i} = H_{val=i}/N^v$

451 represents its probability and  $\overline{A^v}|_{val=i}$  the average area of such void cells. The sample void hence

452 becomes:

$$453 \quad e = \frac{A_{sam}}{A_s} - 1 = \frac{N^v}{N^p} \sum_{i=3} \left( h|_{val=i} \overline{A^v}|_{val=i} / \overline{A^p} \right) - 1 \quad (15)$$

454 where  $N^v$  stands for the total number of void cells.

455 Fig. 13 gives the probability and the average area of void cells with different coordination

456 numbers at the initial and sheared states. It shows clearly that there is a close correlation

457 between the average void cell area and the coordination number. The correlation can be roughly

458 approximated by the polynomial function of power 2, and is found independent of particle

459 friction coefficients. Particles with higher friction coefficients are more likely to form void cells

460 with more constitutive particles, hence the probability of void cells with a larger coordination

461 number is higher. Shearing alters the correlation between  $\overline{A^v}/\overline{A^p}$  and the cell coordination

462 number  $\omega^v$  slightly. Data at 20% deviatoric strain are shown in Fig. 13(b). At the same

463 coordination number,  $\overline{A^v}/\overline{A^p}$  is smaller at the sheared states than that in the initial state,  
 464 indicating the dependence of average void cell area on void cell anisotropy.

465

466 Figure 13 Void cell statistics at different coordination number ( $\mu_p=0.5$ ) (a) Deviatoric strain  
 467 0%; (b) Deviatoric strain 20%.

468

### 469 VOID VECTOR BASED FABRIC QUANTIFICATION AND MATERIAL STRAIN

470 Using the void cell system, the strain of a granular assembly can be considered as the  
 471 volume weighted average of void cell strains. The micro-structural strain definition expresses  
 472 the continuum-scale material strain in terms of particle relative displacements and void vectors  
 473 (Bagi 1996, Kruyt and Rothenburg 1996, Kuhn 1999, Li, Yu et al. 2009), and inspired the  
 474 definition of void vector fabric tensors.

#### 475 The micro-structural strain tensor

476 Following the sign convention defined in (Li, Yu et al. 2009), the compressive strain is  
 477 positive.  $\mathbf{n}(\mathbf{x})$  denotes the normal direction on the boundary surface at point  $\mathbf{x}$ , positive when  
 478 pointing inwards. In two dimensional spaces, the displacement gradient tensor averaged over  
 479 the sample area  $A$  could be evaluated as:

$$480 \quad \bar{e}_{ij} = -\frac{1}{A} \oint_A u_{j,i} dA = \frac{1}{A} \oint_B \mathbf{u} \otimes \mathbf{n} dL \quad (16)$$

481 where  $u_{j,i}$  denotes the displacement gradient and  $L$  is the boundary of the area of interest  $A$   
 482 . The line integral on the right hand side follows the counter-clockwise integration paths over  
 483 the boundary of the area  $A$ . With  $\phi_{ij}$  represents the two dimensional permutation tensor

$$484 \quad \phi_{ij} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad n_i dL = \phi_{ij} dx_j. \text{ Eq. (16) becomes:}$$

485 
$$\bar{e}_{ij} = \frac{\phi_{jk}}{A} \oint_B u_i dx_k = -\frac{\phi_{jk}}{A} \oint_B x_k du_i \quad (17)$$

486 With the material internal structure represented by the void cell system, Eq. (17) can be  
 487 discretized into:

488 
$$\bar{e}_{ij} = -\frac{\phi_{jk}}{A} \sum_{v \in A} \sum_{L^v} x_k \Delta u_i = -\frac{\phi_{jk}}{A} \sum_{v \in A} \sum_{L^v} v_k \Delta u_i \quad (18)$$

489 where  $v_i$  is the vector starting from the contact point to the void cell centre, referred to as the  
 490 void vector. Eq. (18) is a double summation. The inner summation  $\sum_{L^v}^*$  runs over the boundary

491  $L^v$  of void cell  $v$  and  $\sum_{v \in A}^*$  is a summation over all the void cells within the sample area  $A$ . For

492 granular materials, no matter how the sample is divided into sub-domains; the weighted sum of  
 493 local displacement gradient tensors is always the same (Bagi 1993). Denoting

494 
$$e_{ij}^v = -\frac{\phi_{jk}}{A^v} \sum_{L^v} v_k \Delta u_i \quad (19)$$

495 as the local displacement gradient tensor defined on the void cell  $v$ , the sample displacement  
 496 gradient tensor can be written as the area-weighted average over all the void cells:

497 
$$\bar{e}_{ij} = \frac{1}{A} \sum_{v \in A} (A^v e_{ij}^v) \quad (20)$$

498 It is verified that such estimated sample displacement gradient is in good agreement with the  
 499 value obtained from sample boundary.

## 500 **Void vector based fabric quantification**

501 The micro-structural strain definition given in Eq. (18) shows that the key geometrical  
 502 information bridging-up the continuum scale strain and the particle-scale relative displacements  
 503 is void vector, which connects the contact point to the void cell centre. This inspired the void  
 504 vector based fabric tensor definitions (Li and Li 2009). The mathematical treatment has been  
 505 detailed in (Li and Yu 2011) and applied to analyze the contact vectors in the previous session.

506 *Fabric quantification based on void vector probability density*

507 To describe the directional dependence of void vectors, it is of interest to know in each  
508 direction 1) their probability density and 2) their representative (or mean) value. The directional  
509 probability density of void vectors can be quantified in terms of a second rank deviatoric tensor

510 
$$D_{ij}^v = d^v \begin{pmatrix} \cos \phi^v & \sin \phi^v \\ \sin \phi^v & -\cos \phi^v \end{pmatrix} \quad (21)$$

511 following the similar procedure to process information on contact normal and void cell  
512 orientations.

513 *Fabric quantification based on void vector length*

514 As a description of void cell shape in average, the directional dependence of mean void  
515 vector has been characterized in terms of the second rank deviatoric tensor

516 
$$G_{ij}^v = B^v \begin{pmatrix} \cos \beta^v & \sin \beta^v \\ \sin \beta^v & -\cos \beta^v \end{pmatrix}$$
 so that the mean void vector in direction  $\mathbf{n}$  can be approximated

517 as

518 
$$v(\mathbf{n}) = v_0 \left[ 1 + B^v \cos(2\theta - \beta^v) \right] \quad (22)$$

519 where in two dimensional spaces, the unit direction vector is equivalently expressed as  
520  $\mathbf{n} = (\cos \theta, \sin \theta)$ . Based on the mean void vector length, (Li and Li 2009) proposed the void  
521 vector based fabric tensor as:

522 
$$H_{ij}^v = v_0 (\delta_{ij} + G_{ij}^v) \quad (23)$$

523 *The void vector based moment tensor*

524 The void vector based moment tensor can be considered as a combined account of the  
525 anisotropies in void vector density and mean void vector length. It has been used in (Fu and  
526 Dafalias 2015) in structural characterization. The moment tensor can be found as

527  $L_{ij}^v = \langle v_i n_j \rangle = \frac{1}{M} \sum_{\alpha=1}^M v_i^\alpha n_j^\alpha$ . Similar to previous discussions on contact vectors,  $L_{ij}^v$  can be

528 determined from  $D_{ij}^v$  and  $H_{ij}^v$ . In two dimensional spaces,

529 
$$L_{ij}^v = v_0 \left[ \frac{1}{2} (\delta_{ij} + G_{ij}^v) + \frac{1}{4} (D_{ij}^v + D_{im_1}^v G_{jm_1}^v) \right].$$

530 *Internal structure size during shearing*

531 As shearing continues, anisotropy in void vectors develops and is quantified with the two  
532 anisotropy indices  $d^v$ ,  $B^v$ . Both anisotropies are observed to be significant. For all the  
533 simulations in this study, both anisotropies align in the loading direction. And similarity is  
534 observed between their evolutions and those in contact normal density and void cell orientation.  
535 The directional average of void vector length  $v_0$  is regarded as a measure of the void cell size,  
536 and plotted in Fig. 14. It is shown that samples with larger particle friction coefficients have a  
537 larger void vector length, corresponding to larger void cells.

538

539 Figure 14 Directional average of void vector length

540

## 541 **CORRELATION BETWEEN DIFFERENT FABRIC QUANTIFICATIONS**

542 So far, a number of fabric quantifications have been listed in this paper and defined as the  
543 statistical characteristics of contacts, void cells and void vectors, respectively. They are chosen  
544 because of their relevance to material strength and deformation, and formulated based on the  
545 directional statistical theory (Kanatani 1984, Li and Yu 2011). The development of constitutive  
546 model however requires minimizing the number of variable and parameters. It is hence  
547 important to explore the correlations among various fabric quantifications (Fu and Dafalias  
548 2015). The similarities observed in their evolution pattern is encouraging. In this session, the



549 void cell based fabric tensor  $F_{ij}^S$  has been used as a reference to discuss the correlaton among  
550 different fabric quantifications.

551 Among all the fabric tensors, two of them contains informaton reflecting void cell size.  
552 They are the fabric tensor based on void vector length  $H_{ij}^v$ , Eq. (23) and the void cell based  
553 fabric tensor  $F_{ij}^S$ , Eq. (10). The directional averaged void vector length  $\nu_0$  in  $H_{ij}^v$  and the  
554 mean void cell area  $F_{ii}^S = \overline{A^v}$  in  $F_{ij}^S$  are plotted against each other in Fig. 15, showing a strong  
555 correlation in between. It confirms that  $\nu_0$  can be considered as an effective descriptor of  
556 material internal structure size. The correlation is independnt of particle friction coefficient.

557

558 Figure 15 Correlations between internal structure size descriptors

559

560

561

All the fabric tensors contains material anisotropy information. The anisotropy developed  
562 in contact vector length  $G_{ji}^c$  is not elaborated here because its effect is secondary. The  
563 anisotropy index  $d^F$  in the void cell based fabric quantification  $F_{ij}^S$ , Eq. (10) is shown  
564 correlated with other anisotropy indices, including  $d^c$  in contact normal density, Eq. (3),  $d^S$   
565 in void cell orientation, Eq. (9),  $d^v$  in the void vector orientation, Eq. (21) and  $B^v$  in the mean  
566 void vector length, Eq. (23) in Fig. 16. The strong correlation among these anisotropy confirms  
567 the observations made in (Li, Yu et al. 2009, Fu and Dafalias 2015). The anisotropy indices  
568 associated with void vectors are expected to be closely related that in void cells, as confirmed  
569 in Fig. 16(c) & (d). In-depth investigation into structural topology may help to establish the  
570 correlation analytically and to unify the fabric tensor definitions.

571

572 Figure 16 Correlations between the void cell-based anisotropy and other anisotropy indices

573 (a) Contact normal probability density; (b) Void cell orientation; (c) Void vector probability

574 density and (d) Mean void vector length

575

## 576 **DISCUSSION ON STRAIN HETEROGENITY**

### 577 **Observation of deformation pattern**

578 Strain heterogeneity is another important feature of granular materials. The deformation  
579 descriptor in Eq. (19) is defined for each individual void cell and offers a view of spatial  
580 distribution of material deformation. Take the configuration when the void cell system is  
581 constructed as the reference undeformed configuration. The relative displacements occurring  
582 during the subsequent 0.5% deviatoric strain increments are extracted from the DEM  
583 simulations and used to calculate the displacement gradient tensor of each void cell as per Eq.  
584 (19).

585 Fig. 17 shows the local displacement gradients of each void cell when the sample was  
586 sheared from 15% to 15.5% deviatoric strain. The four components of non-affine displacement  
587 gradient tensor, defined as the deviation of the local strain from the sample average  
588 displacement gradient tensor, for the sample with  $\mu_g = 0.5$  are plotted in the separate sub-  
589 figures. It is observed that there are localized banding structures where the strain is much more  
590 significant than the remaining of areas. This is similar to the observation made in (Kuhn 1999)  
591 that slip deformation was most intense within thin obliquely micro bands. Different from the  
592 periodic boundaries used in (Kuhn 1999), the sample boundaries are rigid walls which impose  
593 uniform displacement gradient field. These banding structures do not persist during shearing.  
594 Subsequent loading continuously destroys the existing banding structures and promotes the  
595 formation of new bands in other locations. It is interesting to note that although certain banding  
596 features are commonly observed in the four plots; the patterns for the two shear strain  
597 components are observed to be different from those for the two normal strain components.

598 Furthermore, bands of component  $e_{12}^w$  tend to propagate in the vertical direction while the  
 599 pattern shown by component  $e_{21}^w$  extends in the horizontal direction.

600

601 Figure 17 Patterns of non-affined deformation gradient observed from deviatoric strain

602  $\varepsilon_q = 15\%$  to  $\varepsilon_q = 15.5\%$  ( $\mu_g = 0.5$ ) (a)  $\varepsilon_{11}$  (b)  $\varepsilon_{12}$  (c)  $\varepsilon_{21}$  and (d)  $\varepsilon_{22}$

603

604 The distance between deformation bands is in the order of tens of particle diameters. It is  
 605 several times larger than the internal scale in force chain heterogeneity. Shearing brings about  
 606 continuous formation, development and dissolution of deformation bands, causing  
 607 synchronized swing in the material shear stresses as seen in Fig. 2(a). The developments of the  
 608 force chain heterogeneity and the deformation bands are believed to be critical to the  
 609 deformation and failure of granular systems. It is an area of future research. Considering the  
 610 heterogeneity in material deformation, the sample size may need to be further enlarged to serve  
 611 as a representative element.

## 612 Probability distributions

613 The sample deformation gradient tensor given in Eq. (20) can be interpreted as an integral  
 614 over all the possible local deformation gradient values as

$$615 \quad \bar{e}_{ij} = \int W|_{e_{ij}} e_{ij}^v de_{ij} \quad (24)$$

616 in which  $W|_{e_{ij}} = \frac{1}{A} \lim_{\Delta e_{ij} \rightarrow 0} \frac{\sum A^v|_{e_{ij}^v \in (e_{ij} - \Delta e_{ij}/2, e_{ij} + \Delta e_{ij}/2)}}{\Delta e_{ij}}$  is the area fraction density function. It is the

617 area fraction of void cells whose displacement gradient component  $e_{ij}^v$  falls within the range

618  $e_{ij}^v \in (e_{ij} - \Delta e_{ij}/2, e_{ij} + \Delta e_{ij}/2)$  normalized by the deformation increment  $\Delta e_{ij}$ . Eq. (24) deals with

619 the four components of displacement gradient tensor separately. The Einstein summation over

620 the repeated subscripts doesn't apply here.

621

622 Figure 18 Area fraction density of the four displacement gradient components ( $\mu_g = 0.5$ ,  
623 from  $\varepsilon_q = 15\%$  to  $\varepsilon_q = 15.5\%$ ) (a) normal components and (b) shear components

624

625 Fig. 18 plots the area fraction density function for the four components of displacement  
626 gradient tensor. The data are again taken from the sample with  $\mu_g = 0.5$  when sheared from  
627  $\varepsilon_q = 15\%$  to  $\varepsilon_q = 15.5\%$  as shown in Fig. 17. For all the simulations in this study, the highest  
628 area fraction occurs at zero or near zero deformation. The area fraction decreases quickly as the  
629 magnitude of strain component increases. However, it is worth noting that there exists a large  
630 area fraction where local deformation is much more prominent than the continuum scale  
631 average 0.5%. Although the samples are loaded in the biaxial mode, significant shear strains  
632 are observed, indicating rigid body rotation or deformation deviated away from the vertical  
633 direction are important deformation mechanisms in local void cells. The continuum-scale  
634 deformation is of small magnitudes because there are significant portions of positive as well as  
635 negative strain components which compensate each other.

636 Particle friction coefficient has a significant influence on deformation distribution.  
637 Samples of smooth particles show more dispersed but more significant void cell deformations.  
638 Fig. 19 presents the probability distribution of void cell deformations by plotting the area  
639 fraction of positive and negative normal strains and the averages of positive and negative shear  
640 strain components respectively. The shape of function  $W|_{e_{ij}}$  for the two shear components is  
641 symmetric with respect to  $x = 0$ , corresponding to the observation that the area fractions for the  
642 positive and negative shear components are around 50%, although not plotted here.

643

644 Figure 19 Development of void cell strains (a)  $\mu_p = 0.0$  (b)  $\mu_p = 0.5$  and (c)  $\mu_p = 10.0$

645

646 With increase in particle friction coefficient, the area fraction with positive  $e_{22}$  and  
647 negative  $e_{11}$  increase as shown in Fig. 19. For frictionless particles  $\mu_g = 0.0$ , there are  
648 extensive and significant deformations observed in all void cells. Around 55% of sample area  
649 goes through positive  $e_{22}$  or negative  $e_{11}$  which is only slightly larger than the area fraction 45%  
650 for negative  $e_{22}$  or positive  $e_{11}$ . The average magnitudes of normal strain components are  
651 around 2%, and of shear strain components around 4%. However, with larger particle friction  
652 coefficient, for example, in the case  $\mu_g = 0.5$ , there is nearly 70% percent of area with positive  
653  $e_{22}$  or negative  $e_{11}$ . The average magnitudes of normal strain components are around 1% with  
654 a slightly larger value for shear strain components. The average magnitudes are observed to  
655 increase slightly at the extremely high particle friction coefficient  $\mu_g = 10.0$  indicating the  
656 deformation distribution gets slightly dispersed. Differences have also been observed in  
657 deformation at small strain levels. For higher particle friction coefficients, the local void cell  
658 deformation is more uniform and close to the continuum-scale average deformation, i.e.,  
659 smaller non-affine deformation. And it takes a larger strain level to develop into the deformation  
660 patterns at the critical states.

661 There is however not yet a clear conclusion on what fabric information affects strain  
662 heterogeneity and the consequent impact on material deformation. The relative displacement  
663 between particles may result from different combinations of contact sliding and rolling  
664 (Iwashita and Oda 1998, Kuhn and Bagi 2004). More research in studying local particle  
665 rearrangement and contact movement (Nguyen, Magoaric et al. 2012) is needed.

## 666 CONCLUDING REMARKS

667 This paper studies the behavior of granular material as the collective response of void cells  
668 based on the multi-scale data obtained from a series of numerical simulations with different  
669 particle friction coefficients. More anisotropic structures have been formed in more frictional  
670 materials, and they can support larger contact force anisotropies. The difference in particle  
671 friction coefficient also causes significant difference in internal structure size. More frictional  
672 particles tend to form less but larger void cells, leading to a larger sample void ratio.

673 The definition of fabric tensor requires 1) identifying the key aspect of material internal  
674 structure and 2) understanding its influence on the stress-strain responses. Three groups of  
675 fabric tensor have been covered in this paper. The first one is based on contact vectors. Fabric  
676 tensors based on contact normal density and the contact vector moment tensors are identified  
677 as effective indices associated with material strength, and their impact on material stress  
678 quantified by the SFF relationship. The second group is defined on void cell characteristics.  
679 The fabric tensor based on the area moment of inertia  $S_{ij}^v$  has been proposed to characterize  
680 the individual void cell geometry and their statistical average as material fabric tensor, Eq. (10).  
681 Fabric tensors have been defined based on the void cell orientation and as the statistical average  
682 of void cell characteristics. Material dilatancy can be interpreted by tracing the void cell  
683 statistics during shearing. For frictionless particles, shearing doesn't change the void cell size  
684 much. However, for high friction particles, shearing will form larger void cells, causing dilative  
685 material responses. The micro-structural strain definition given in Eq. (18) suggests the void  
686 vector based fabric tensor definitions could be potential candidates when studying material  
687 deformation, including those based on void vector probability density and the directional  
688 distribution of mean void vectors.

689 Correlations among various fabric quantifications have been explored. The mean void  
690 vector length and the mean void cell area are parameters quantifying the internal structure size,

691 and strongly correlated with each other. Anisotropy indices defined based on contact normal  
692 density, void vector density, void vector length and void cell orientation are found effective in  
693 characterizing loading-induced anisotropy. They are also closely correlated. The fabric tensor  
694 definitions, such as the fabric tensors defined on the void vector length and that based on  
695 individual void cell characteristics, are advantageous for reflecting both the internal structure  
696 size and material anisotropy. In-depth investigation on structural topology may help establish  
697 the correlation among different fabric descriptors and unify the fabric tensor definition.

698 Deformation of granular materials is highly heterogeneous. The deformation of individual  
699 void cells has been calculated and the local deformation is shown to be much more significant  
700 than the continuum-scale average strain. Deformation bands have been observed. With sample  
701 boundaries formed by rigid planar walls, shearing continuously destroys the existing banding  
702 structures and promotes the formation of new bands in other locations. The distance between  
703 these deformation bands is in the scale of tens of particle diameters. Its relation to and impact  
704 on material deformation is an area of future investigation.

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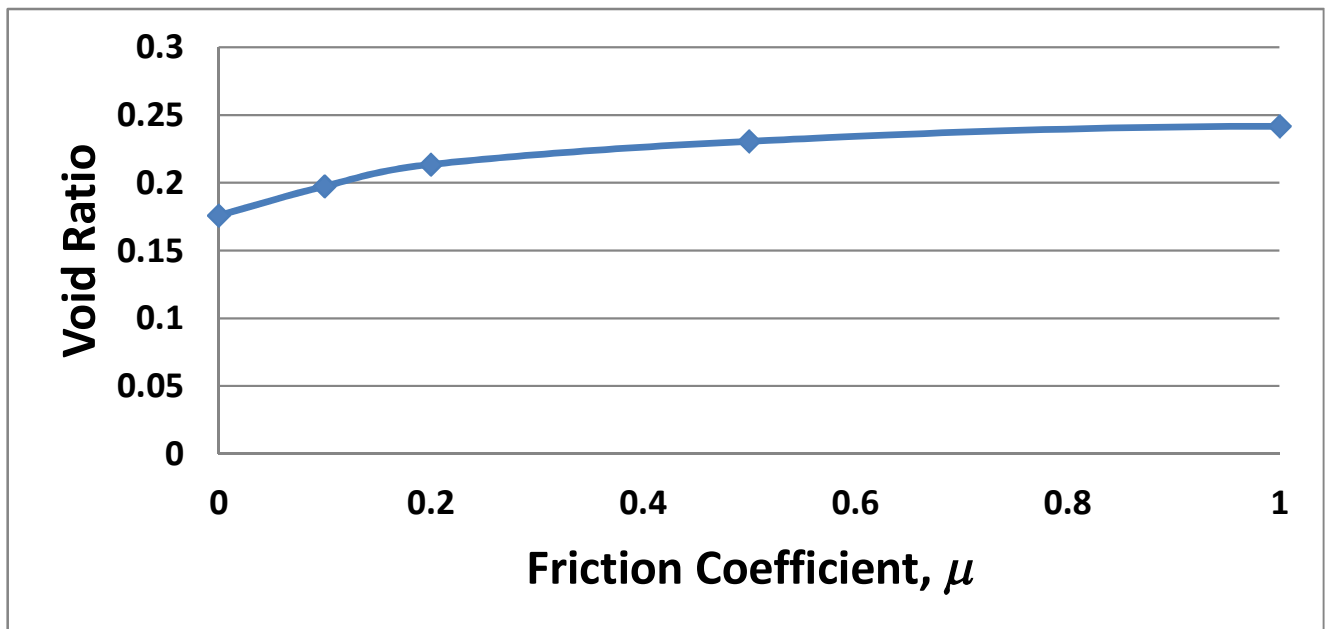
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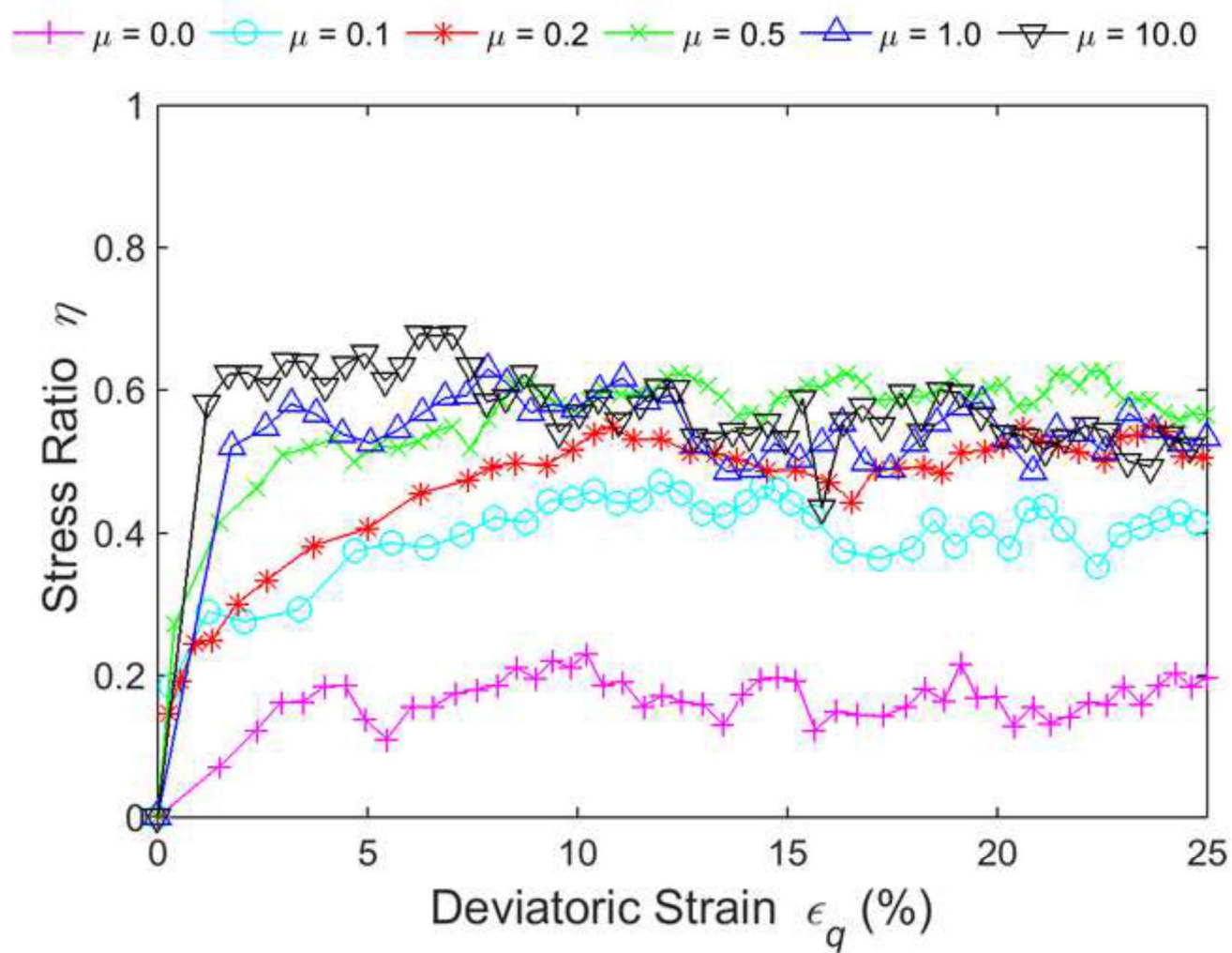
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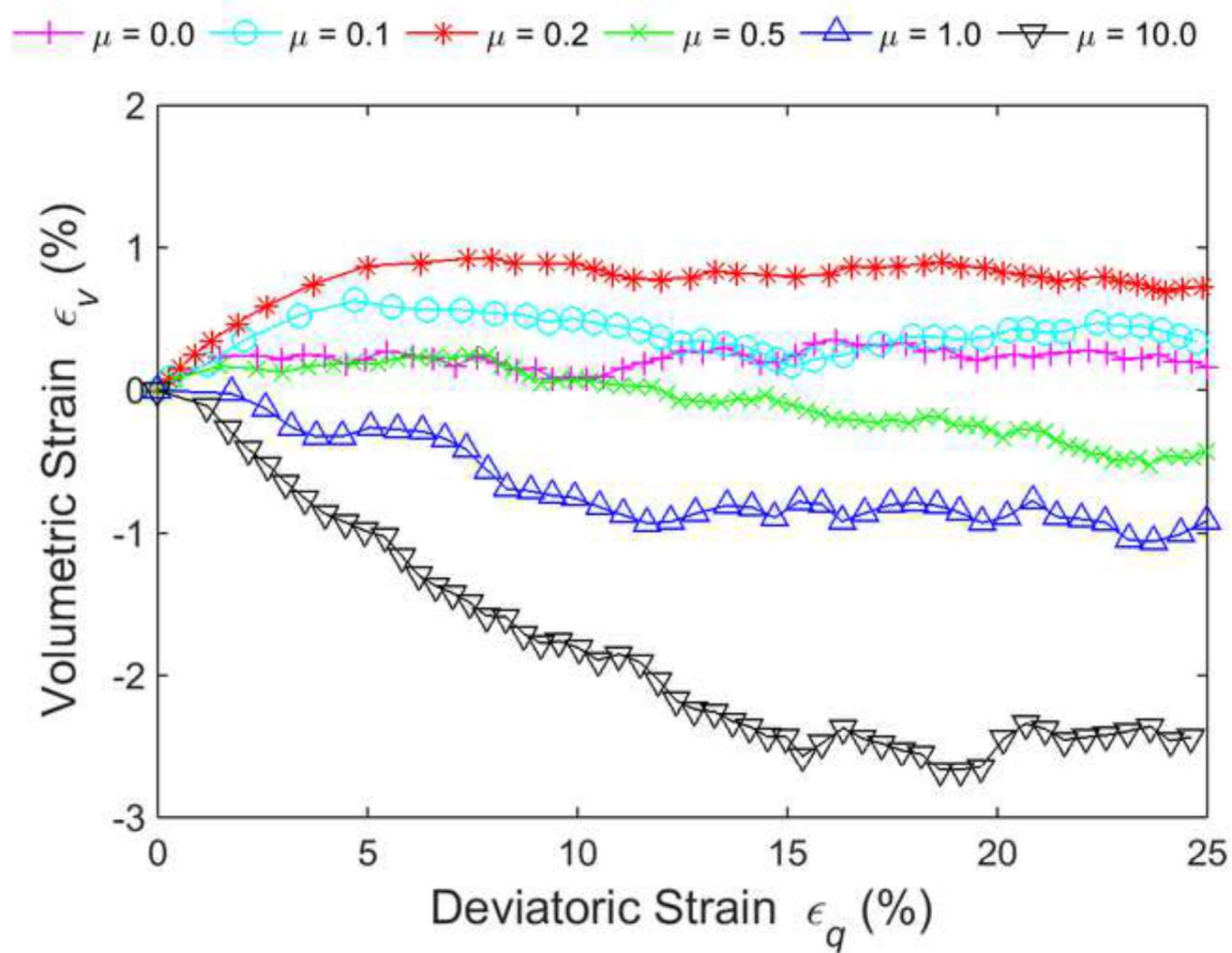
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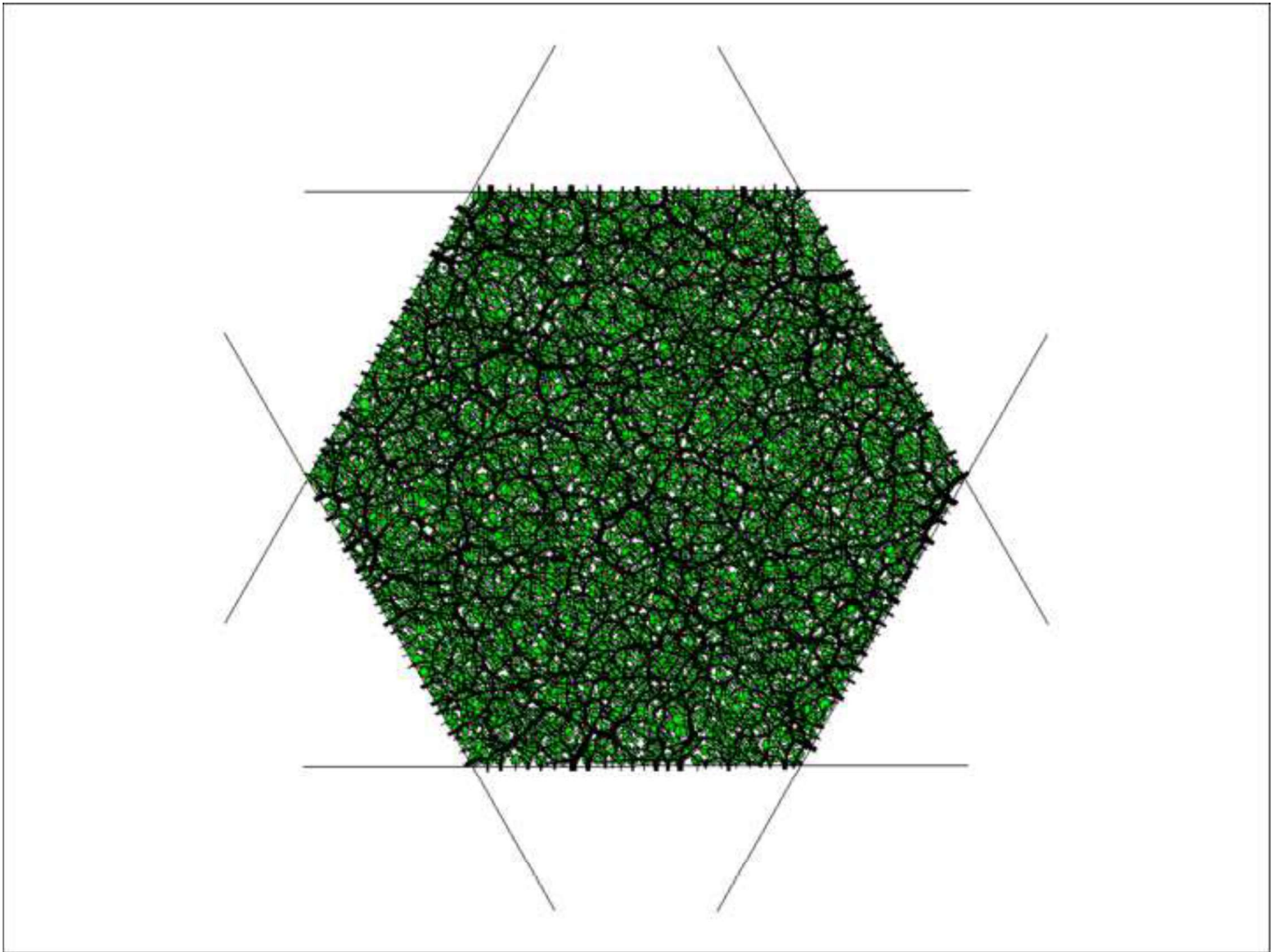
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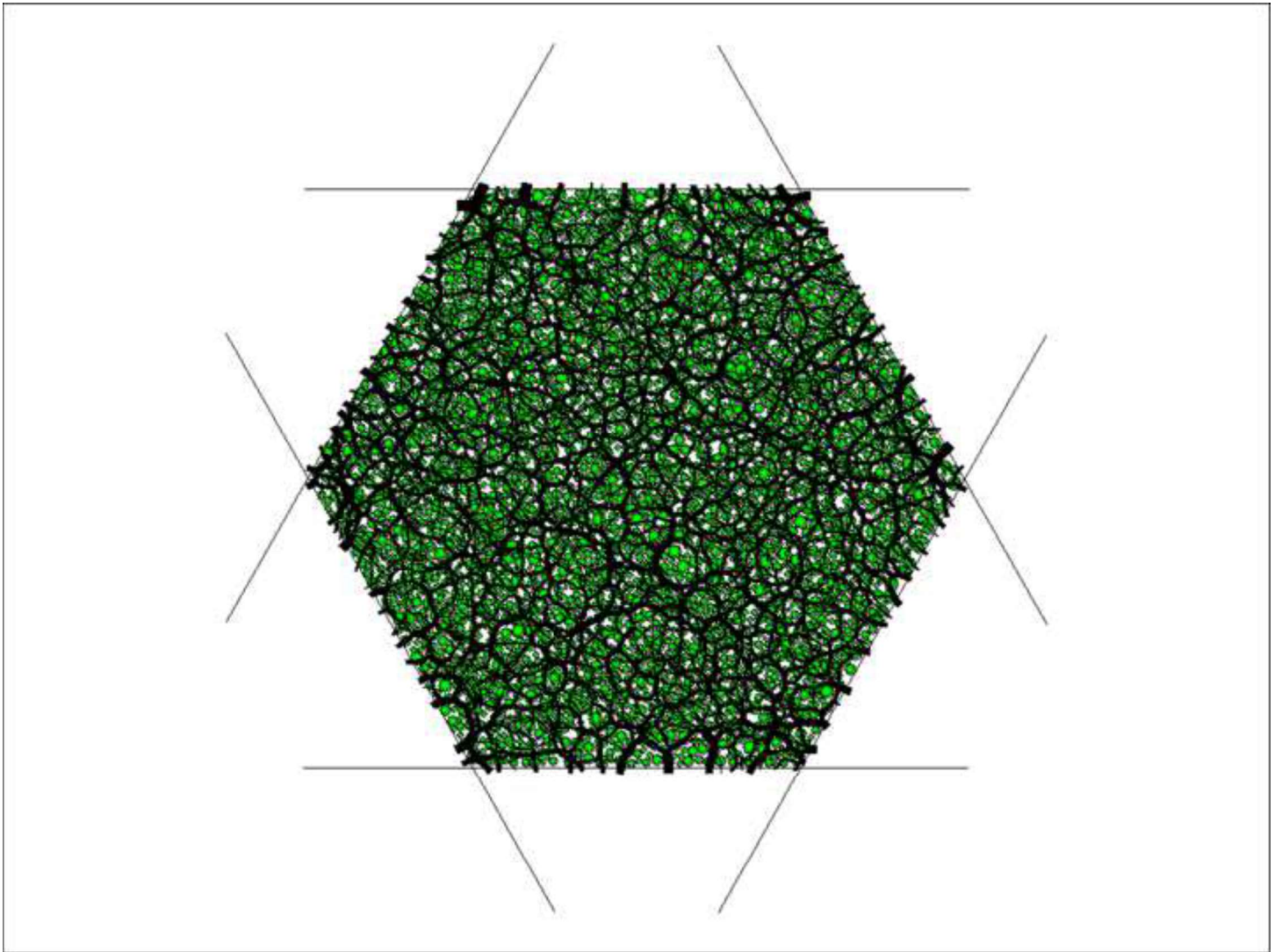


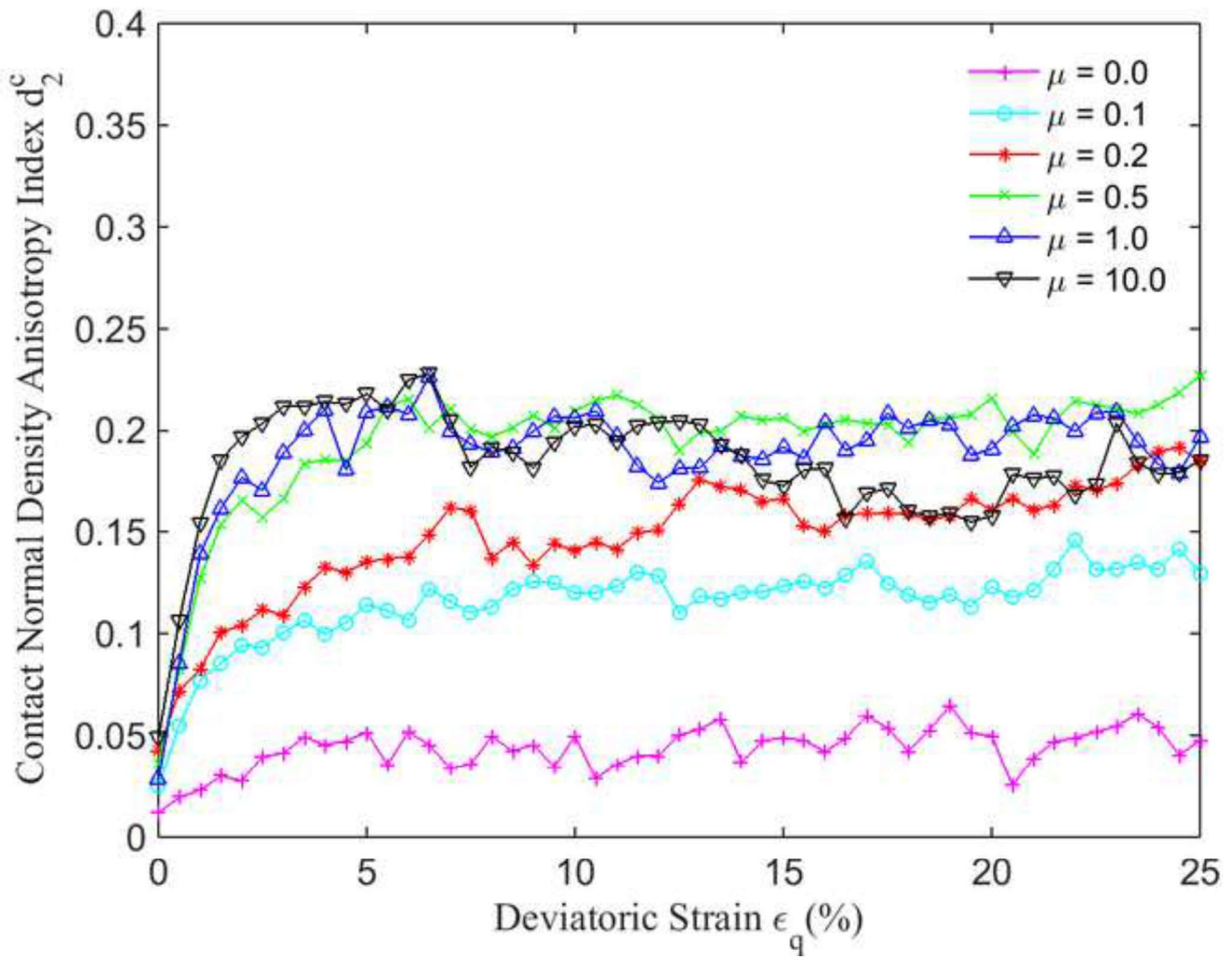


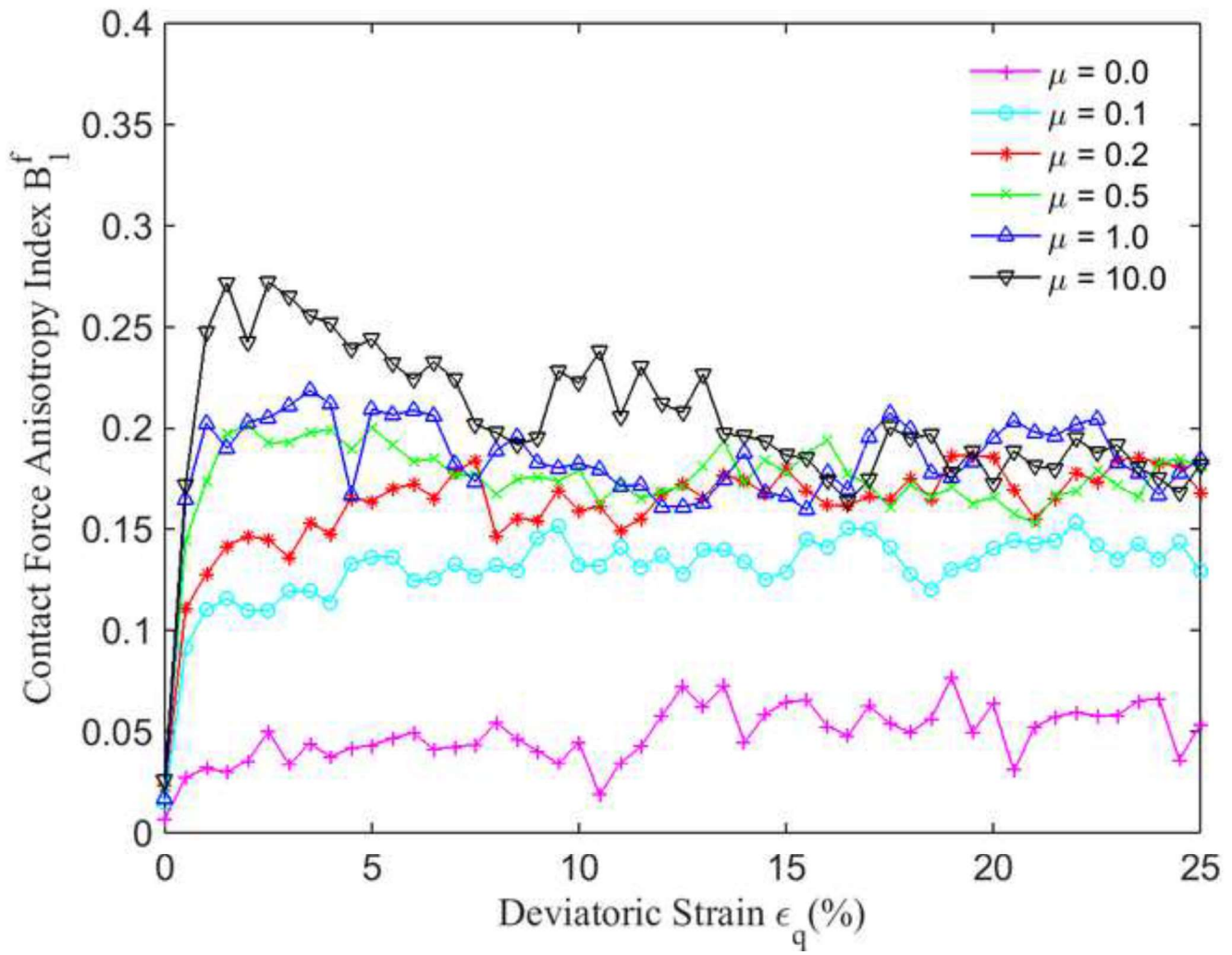
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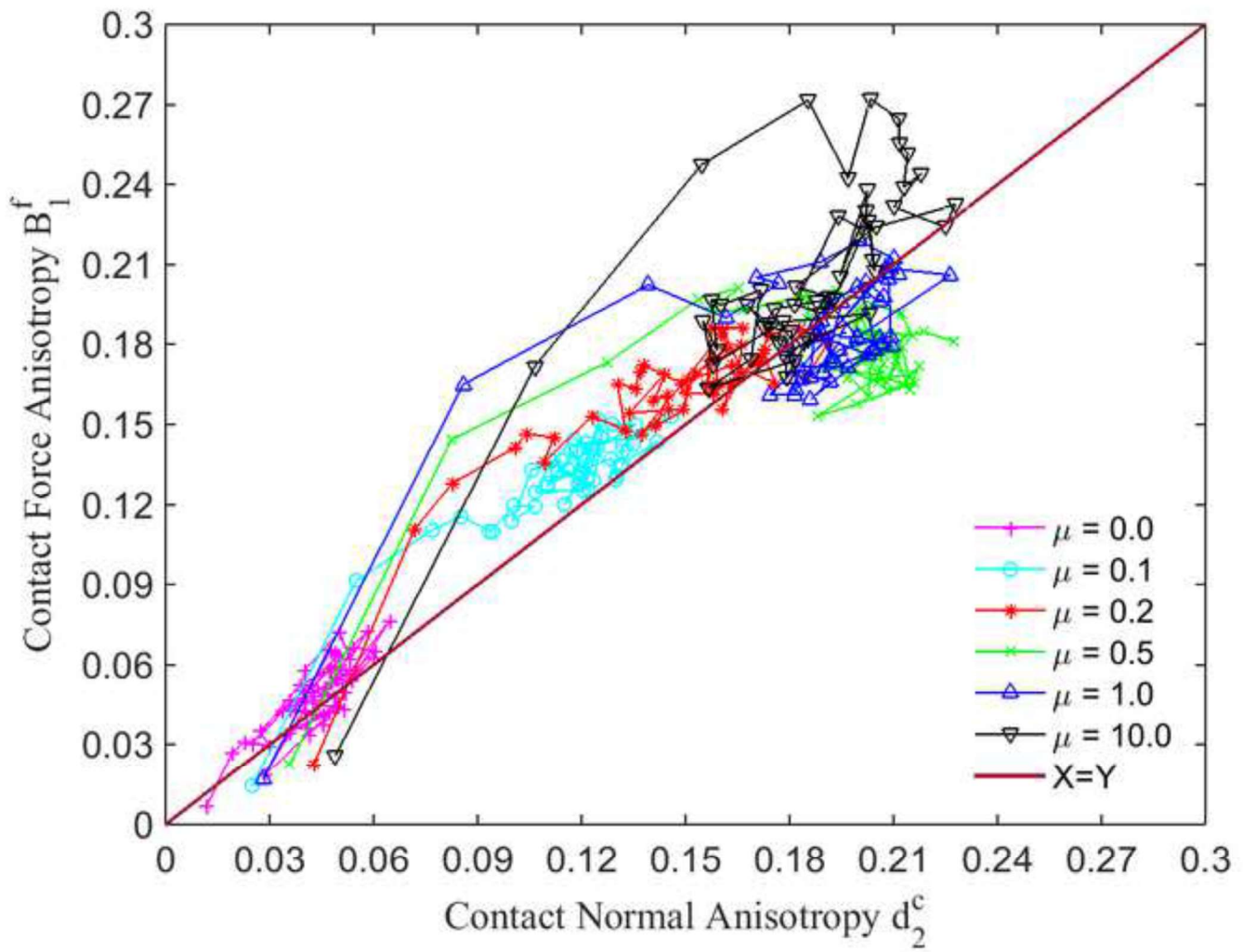
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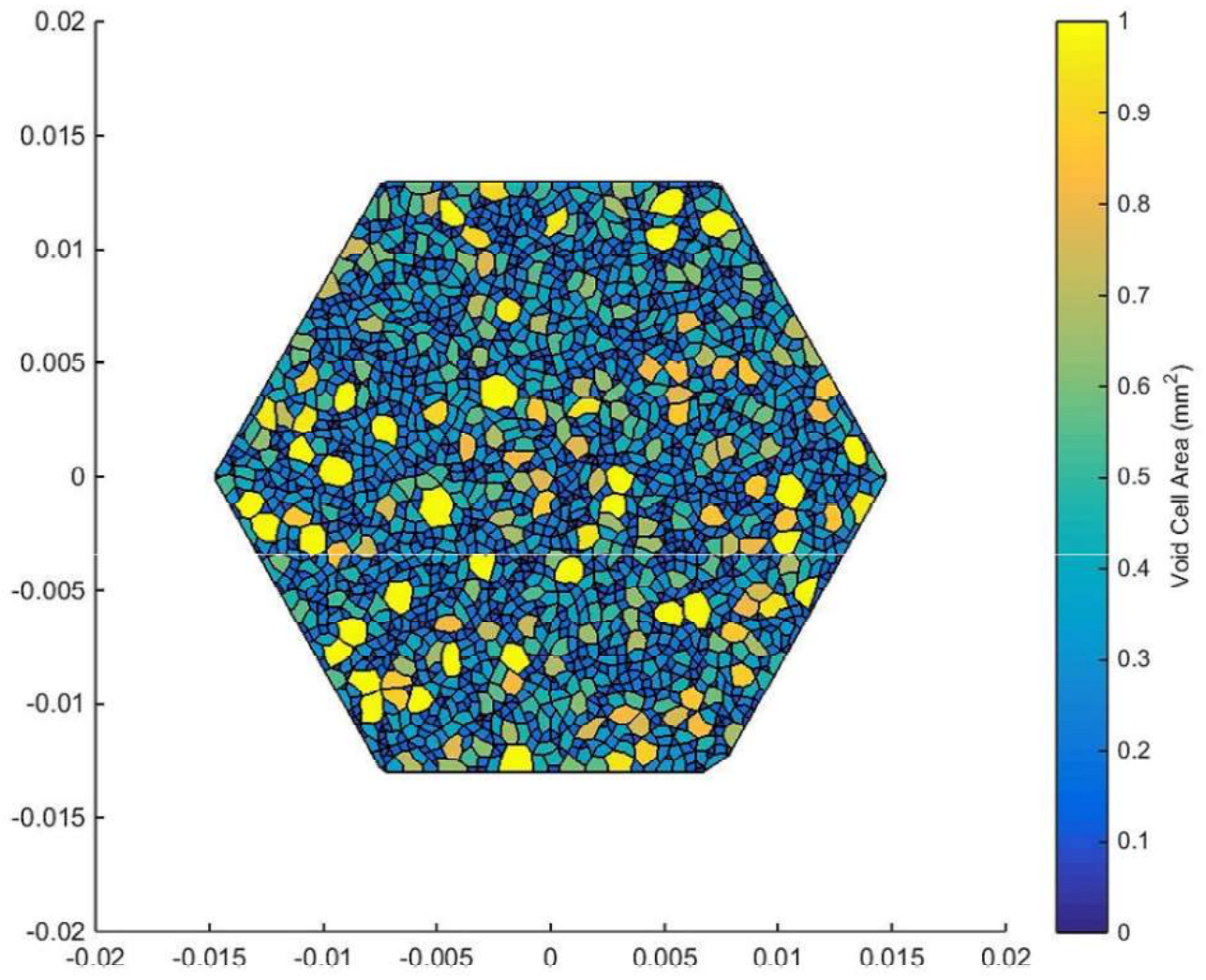






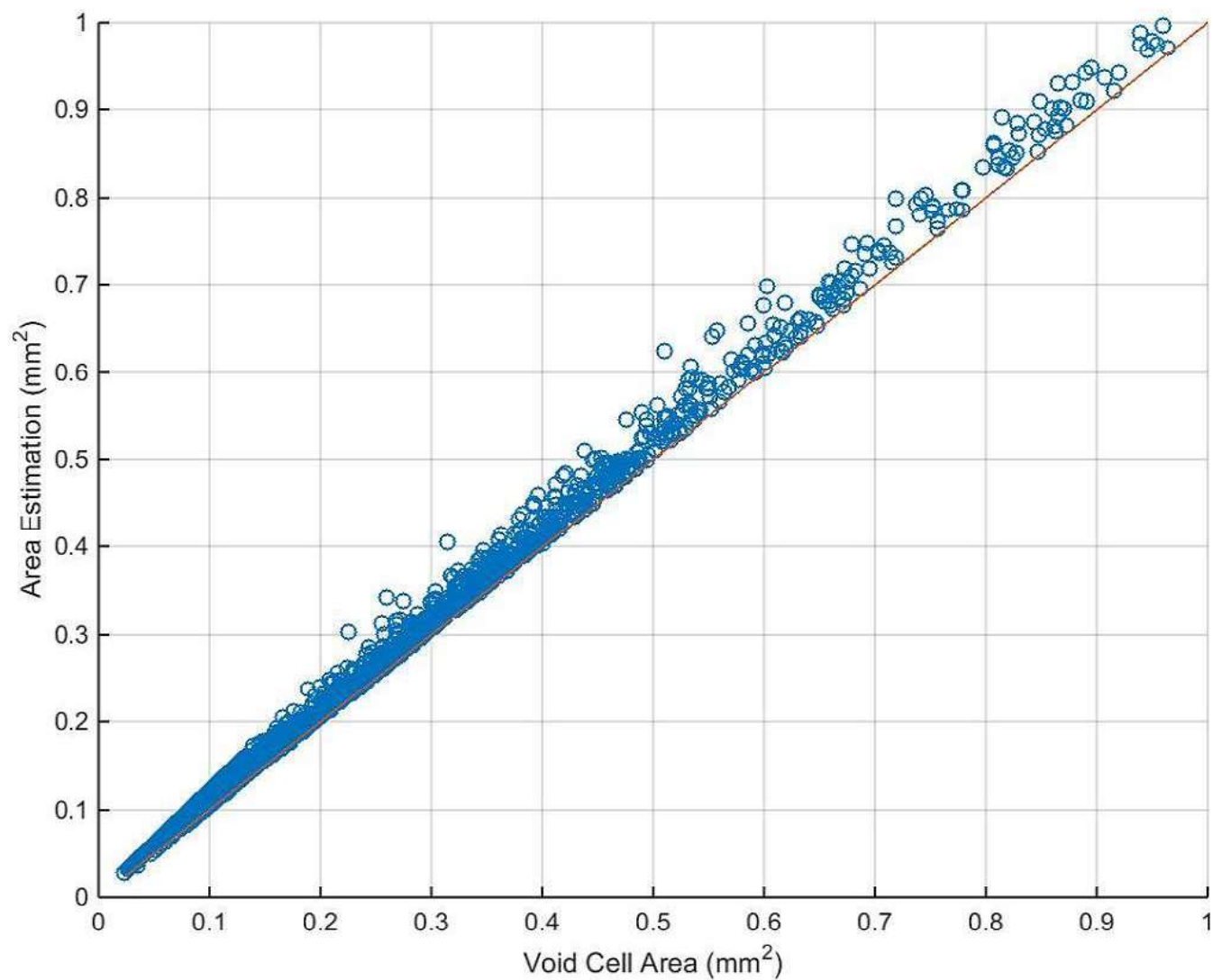
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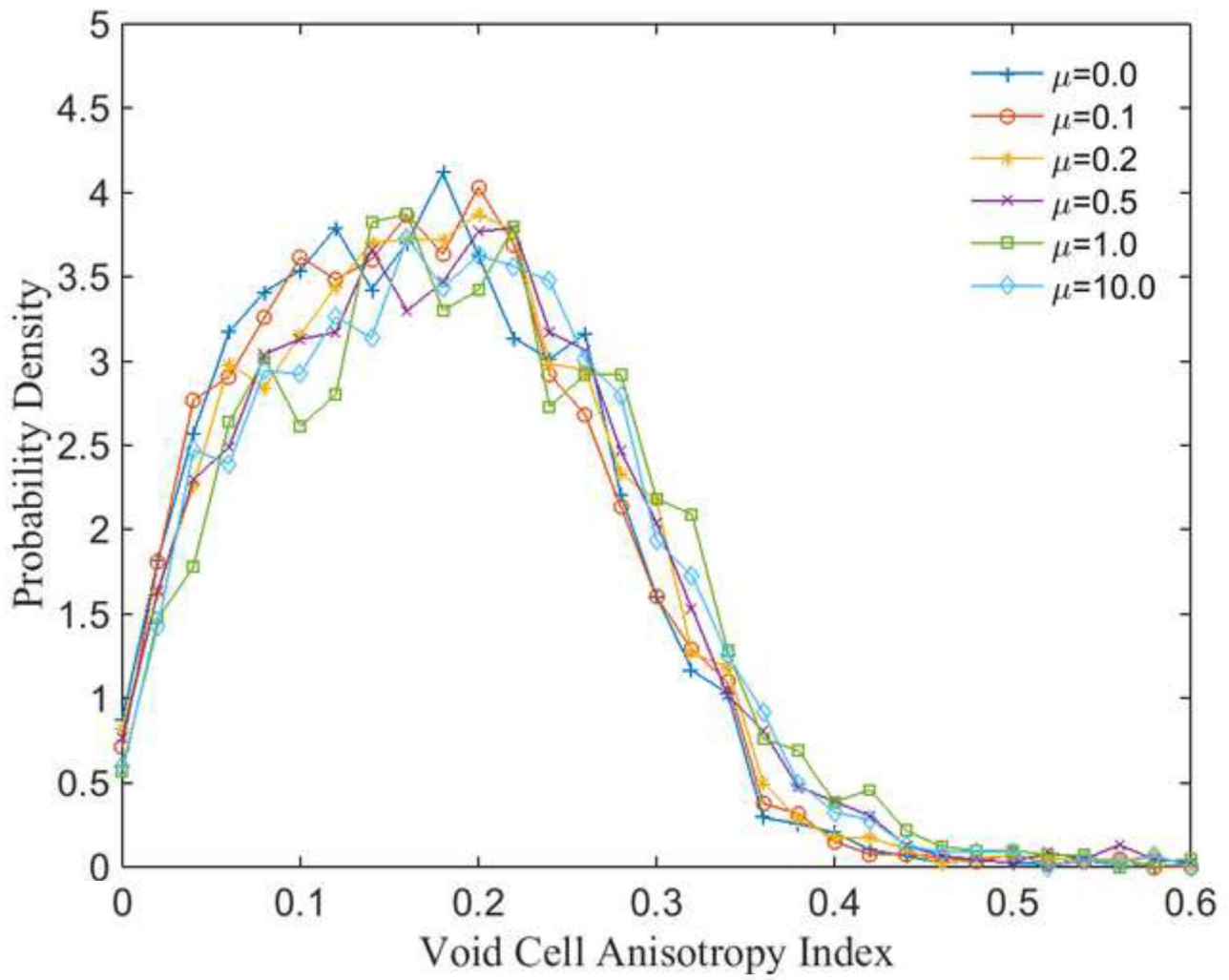
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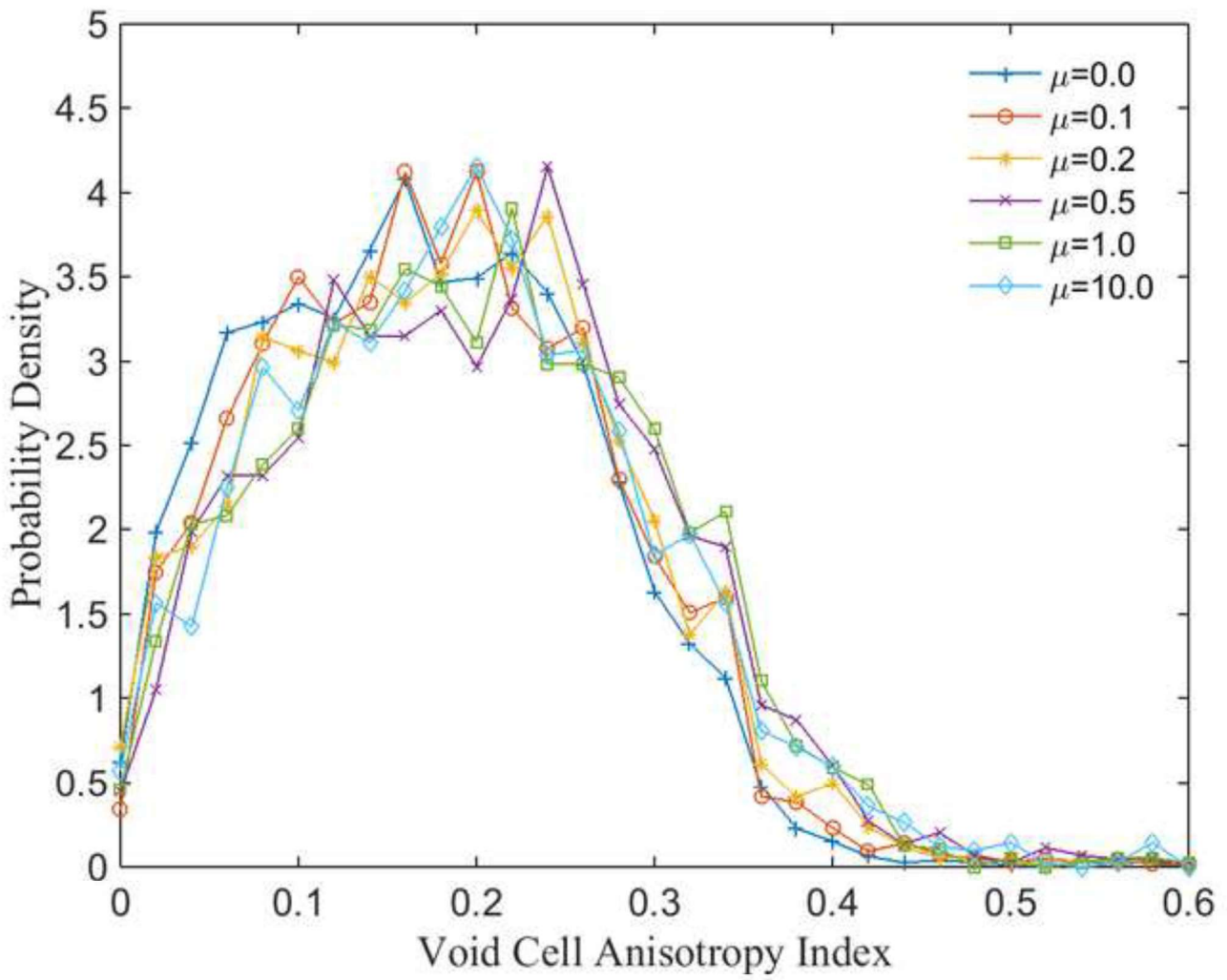


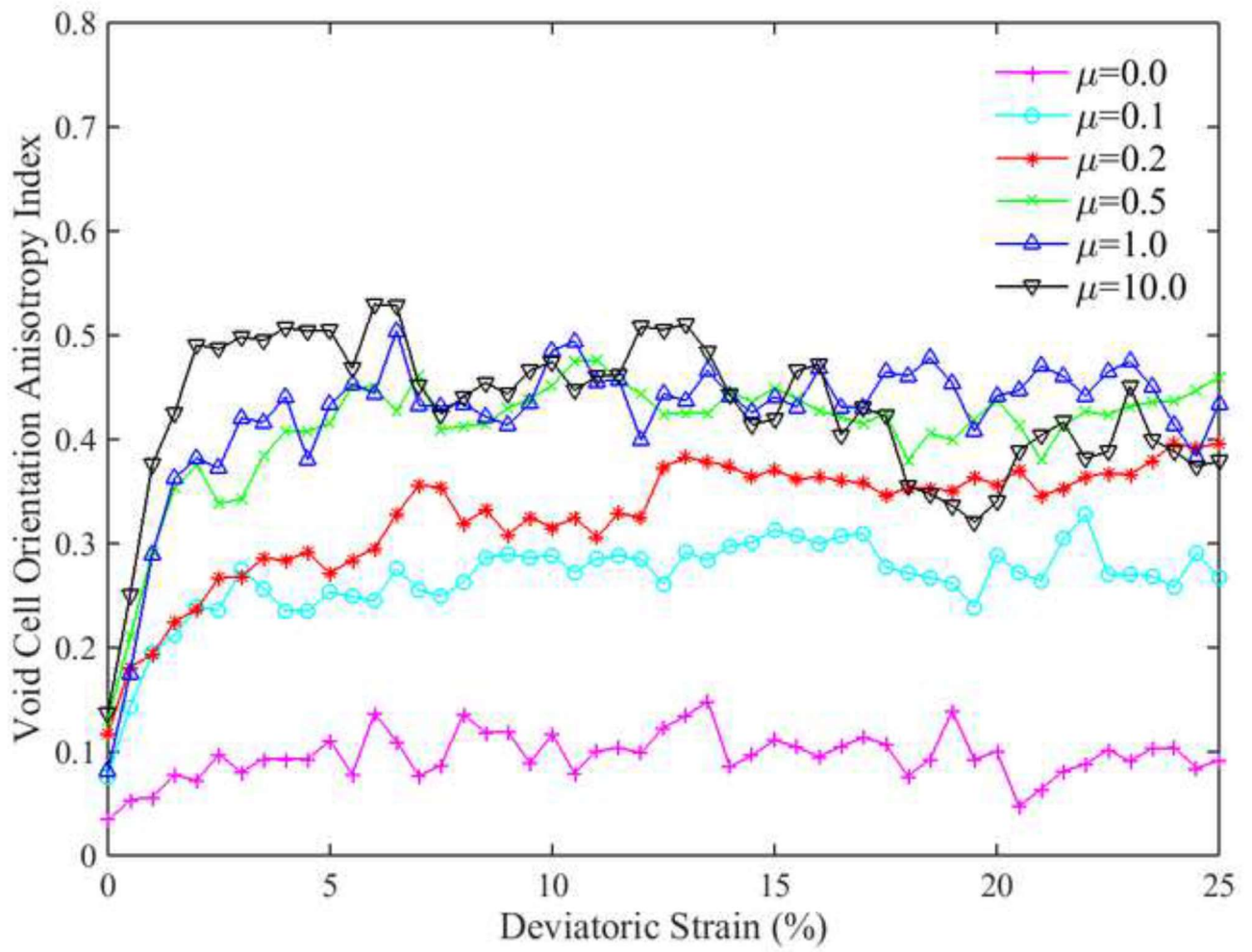
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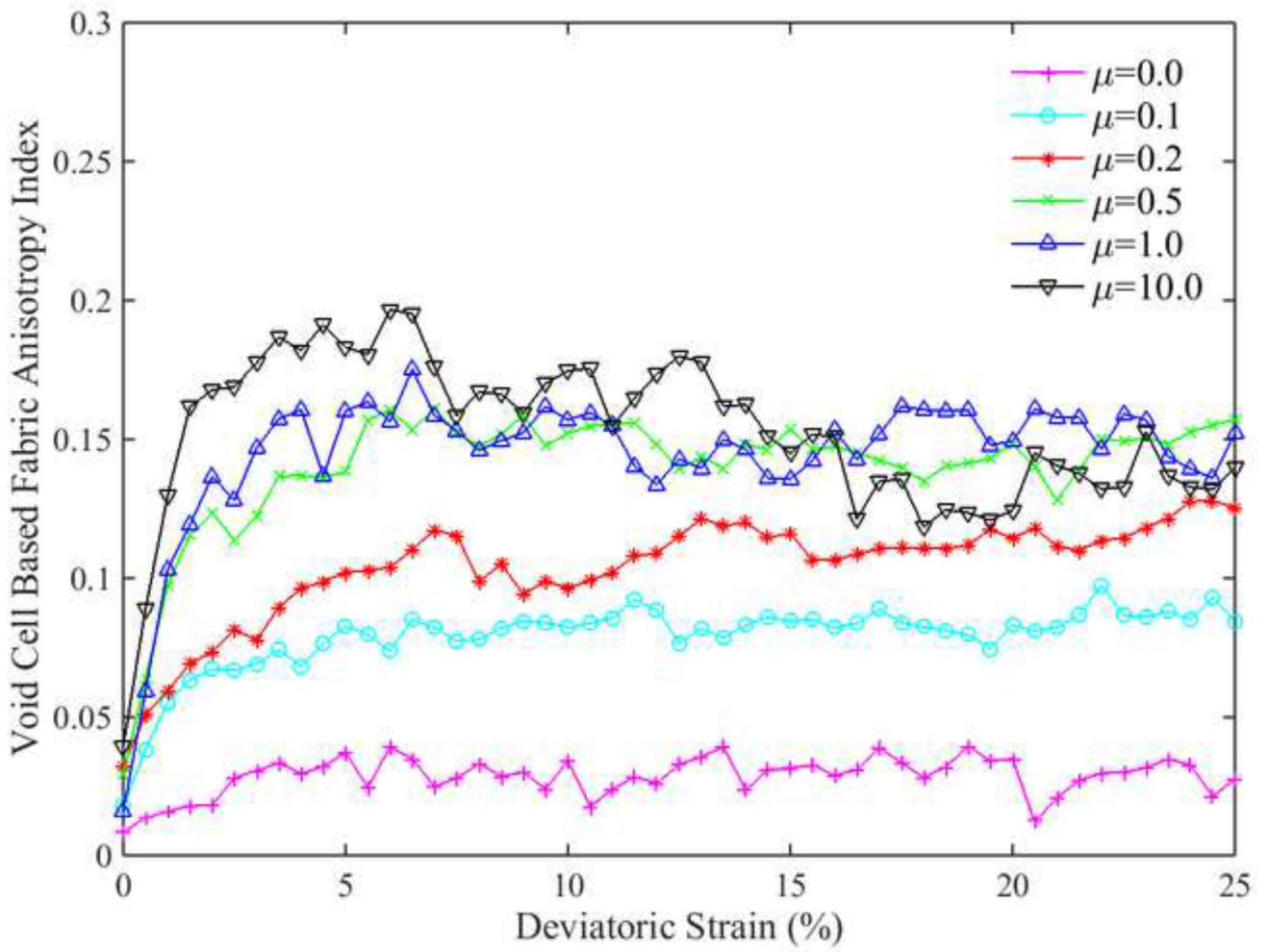
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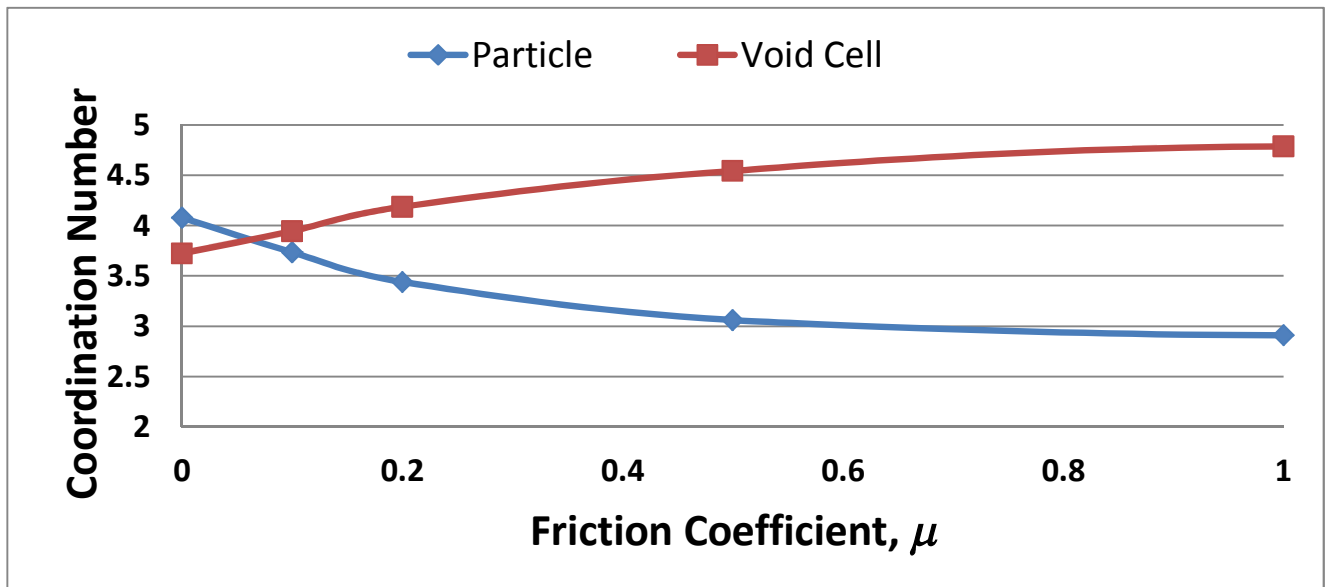




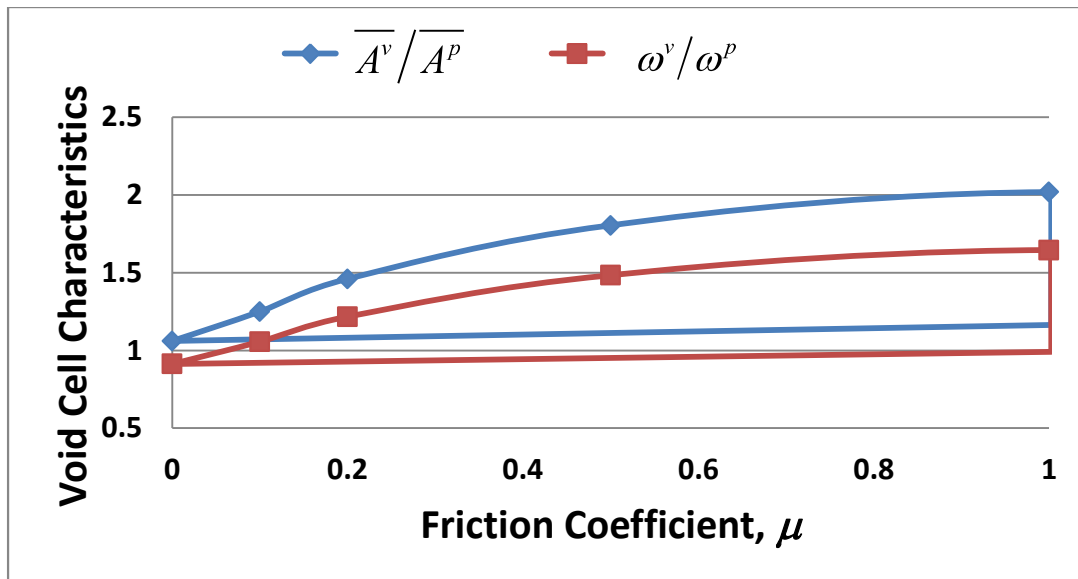


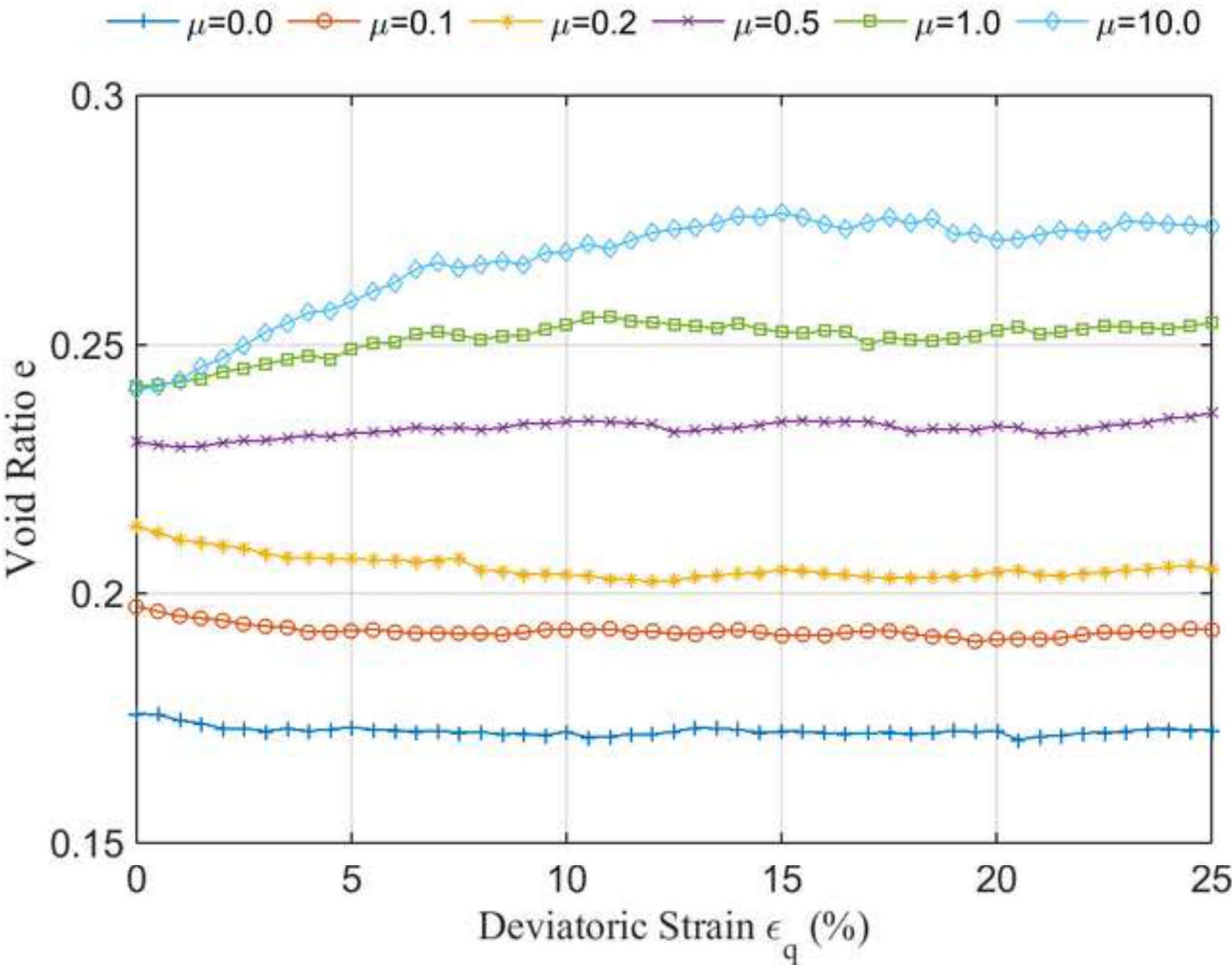


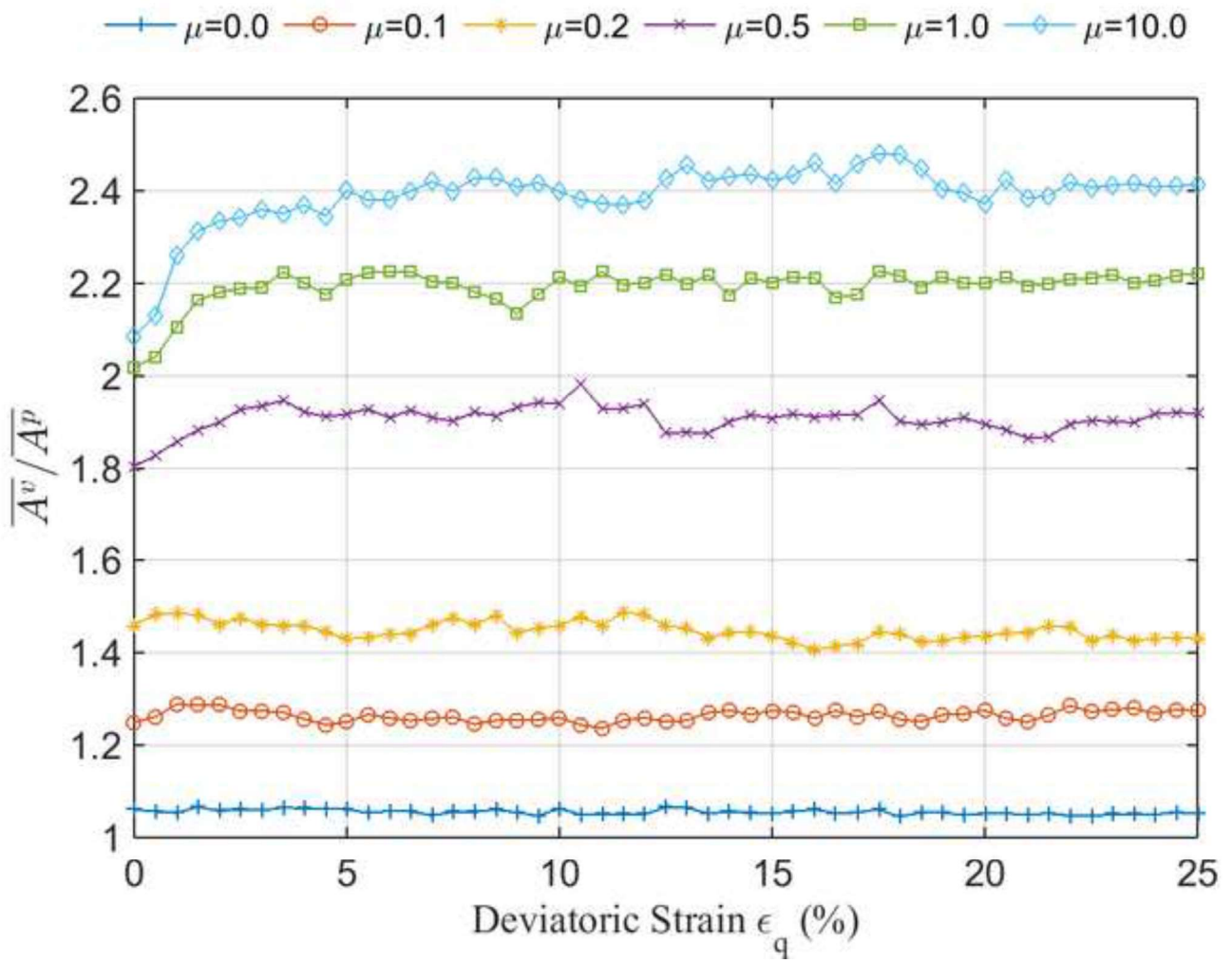


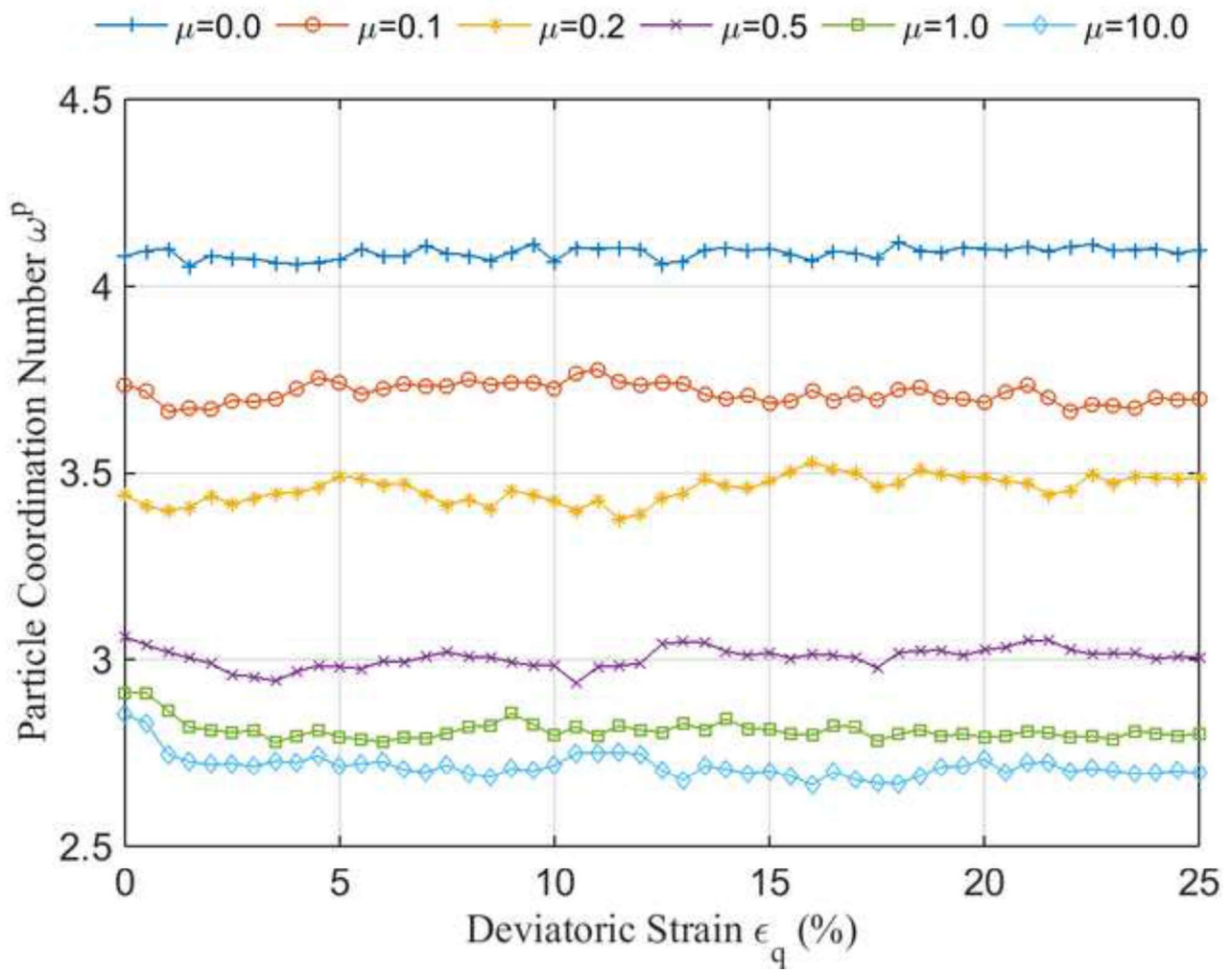


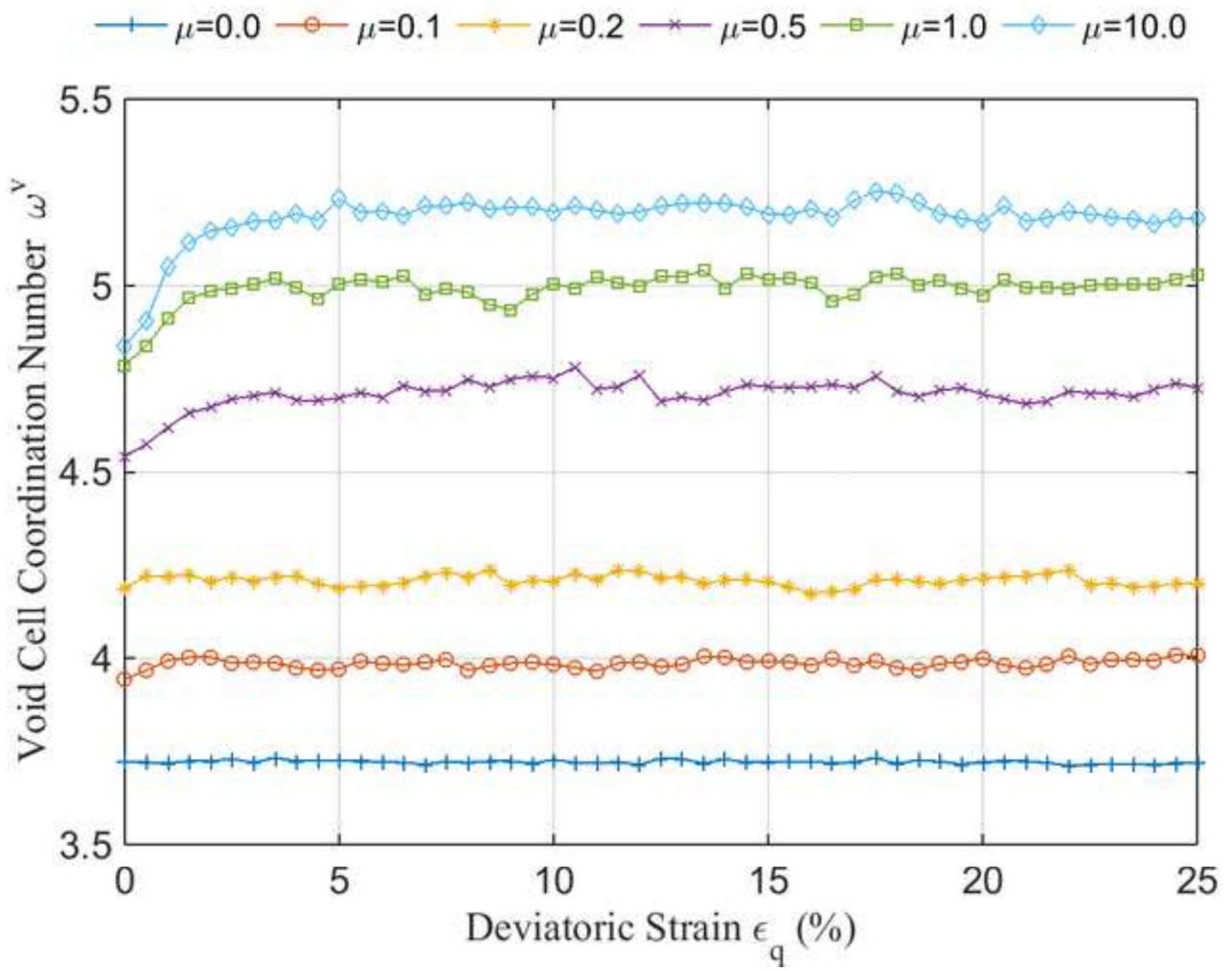


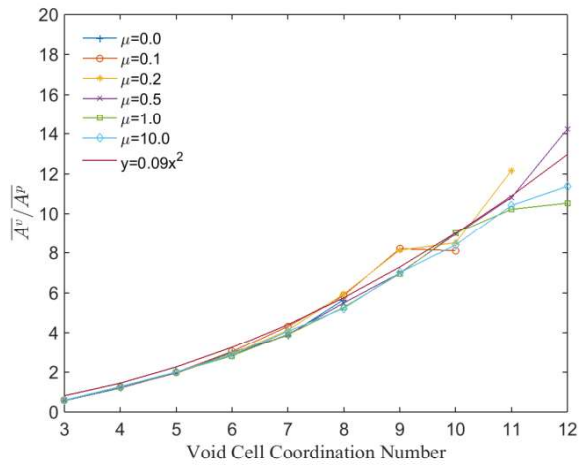
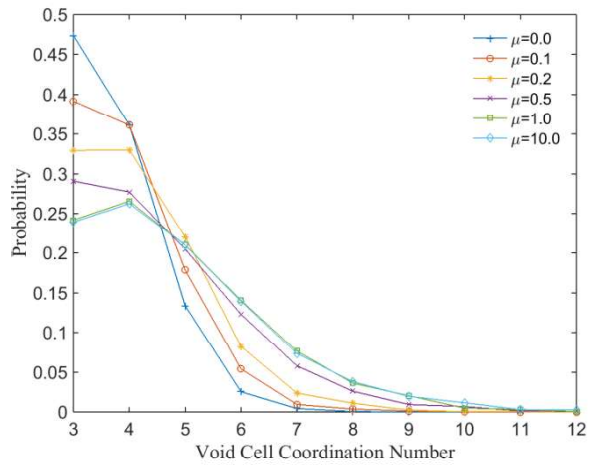


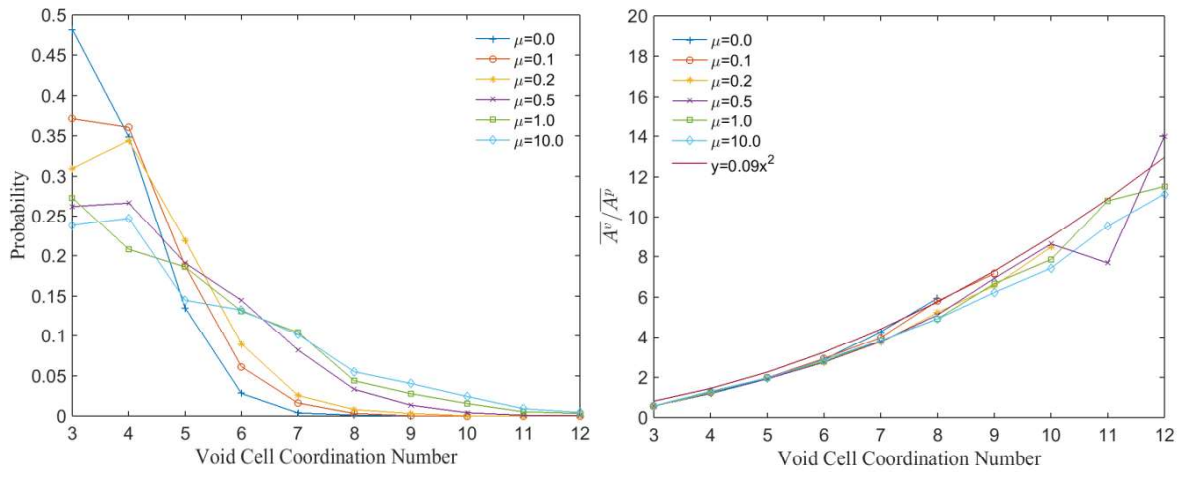


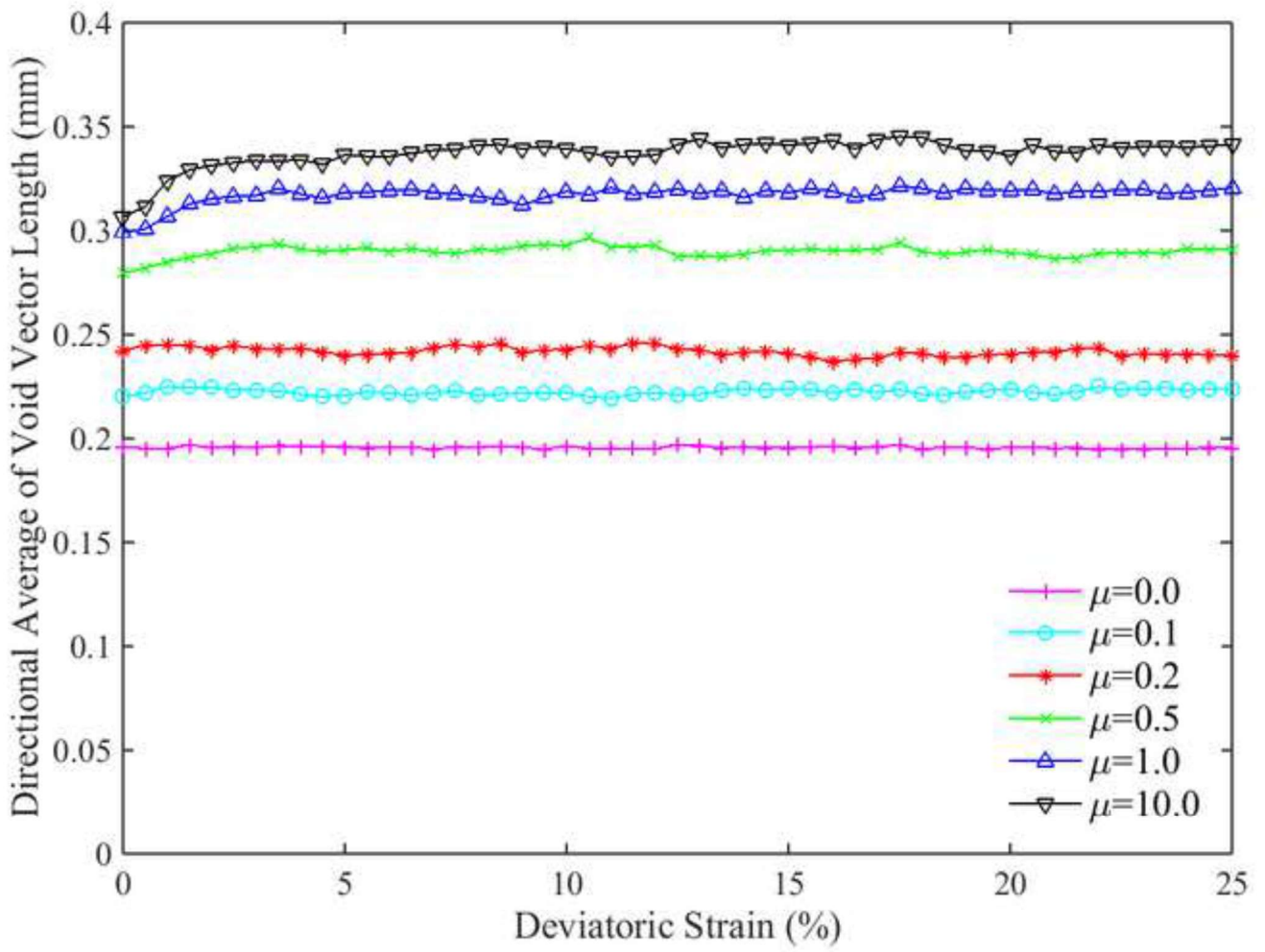




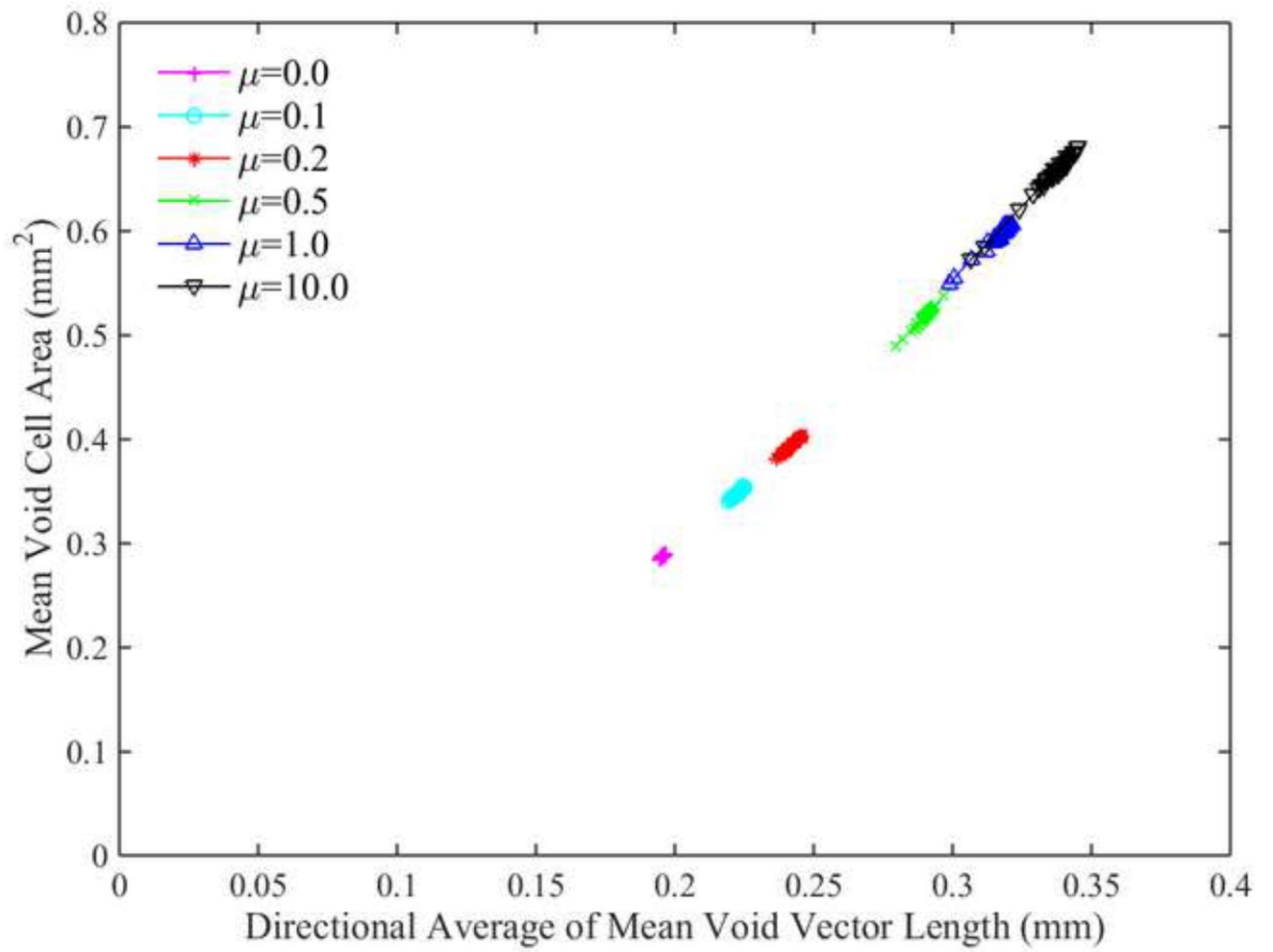


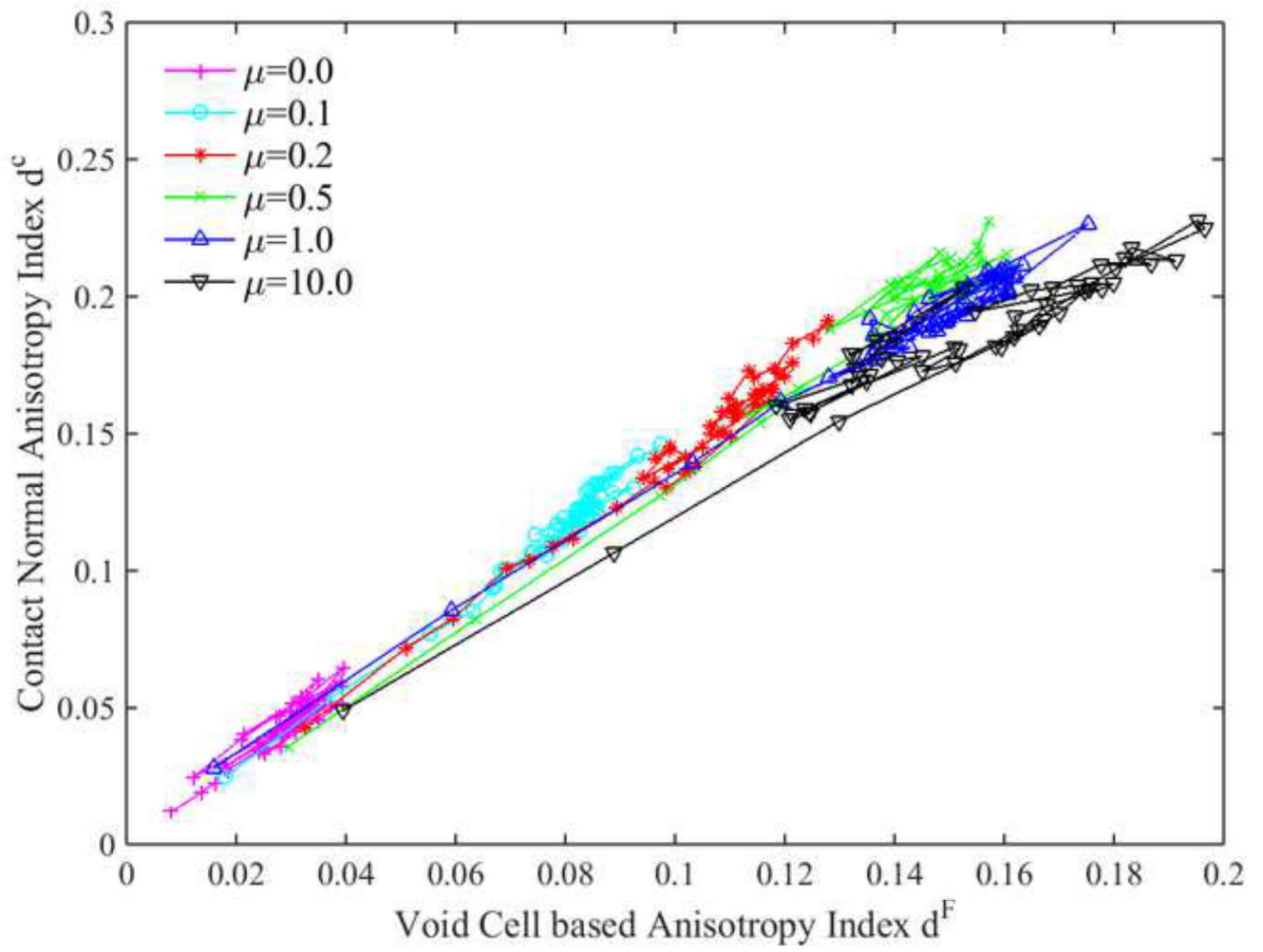


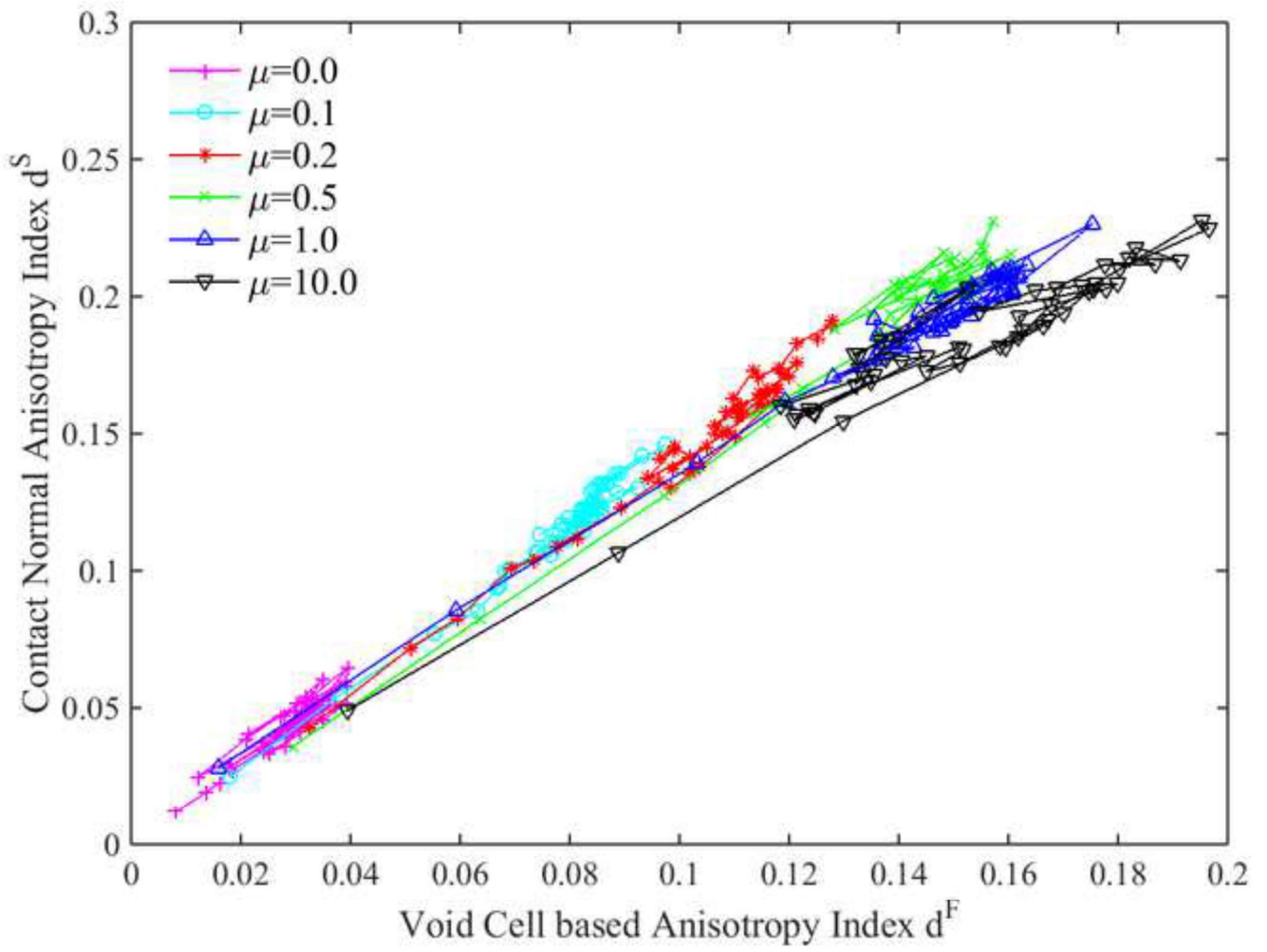


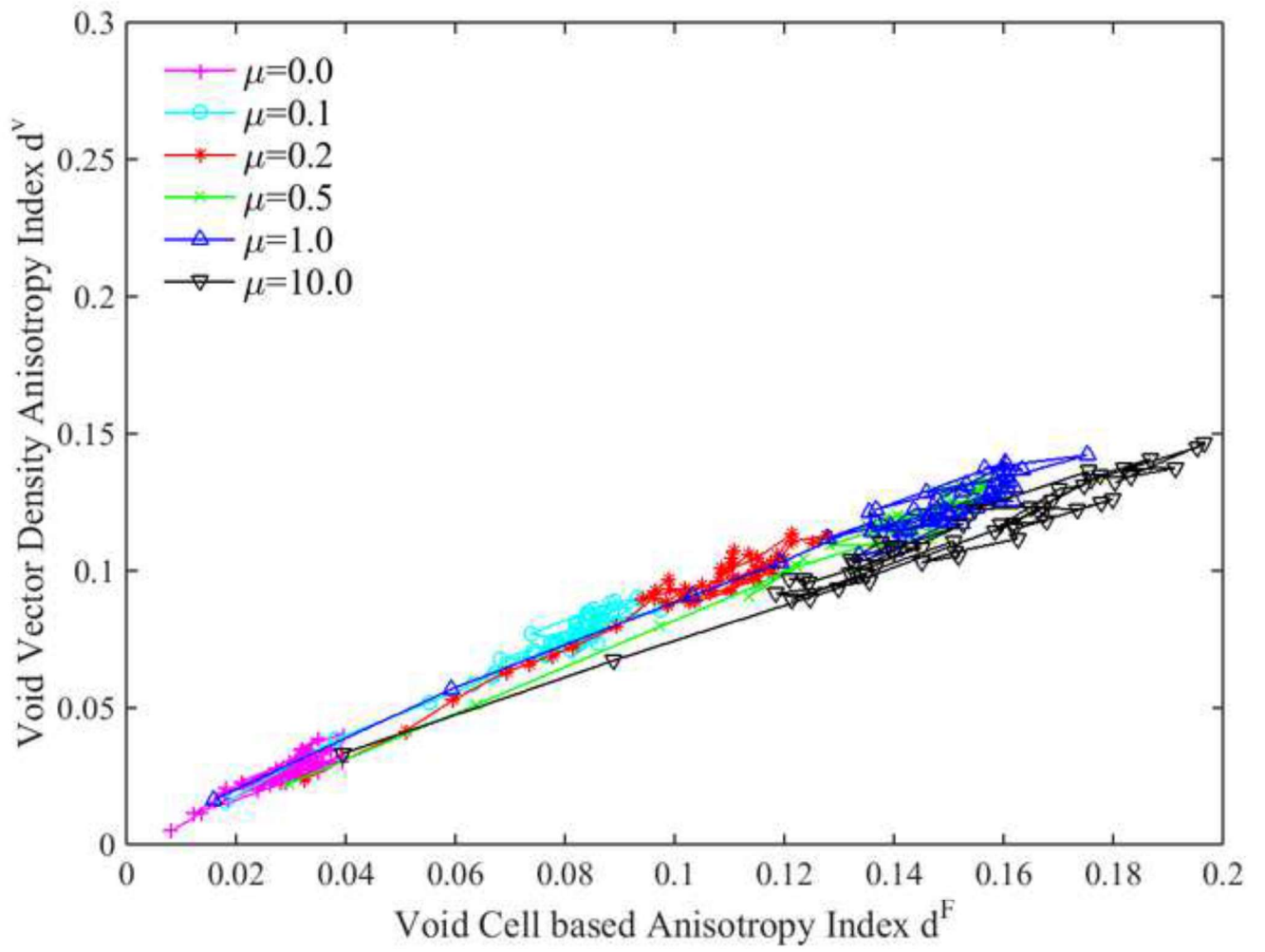


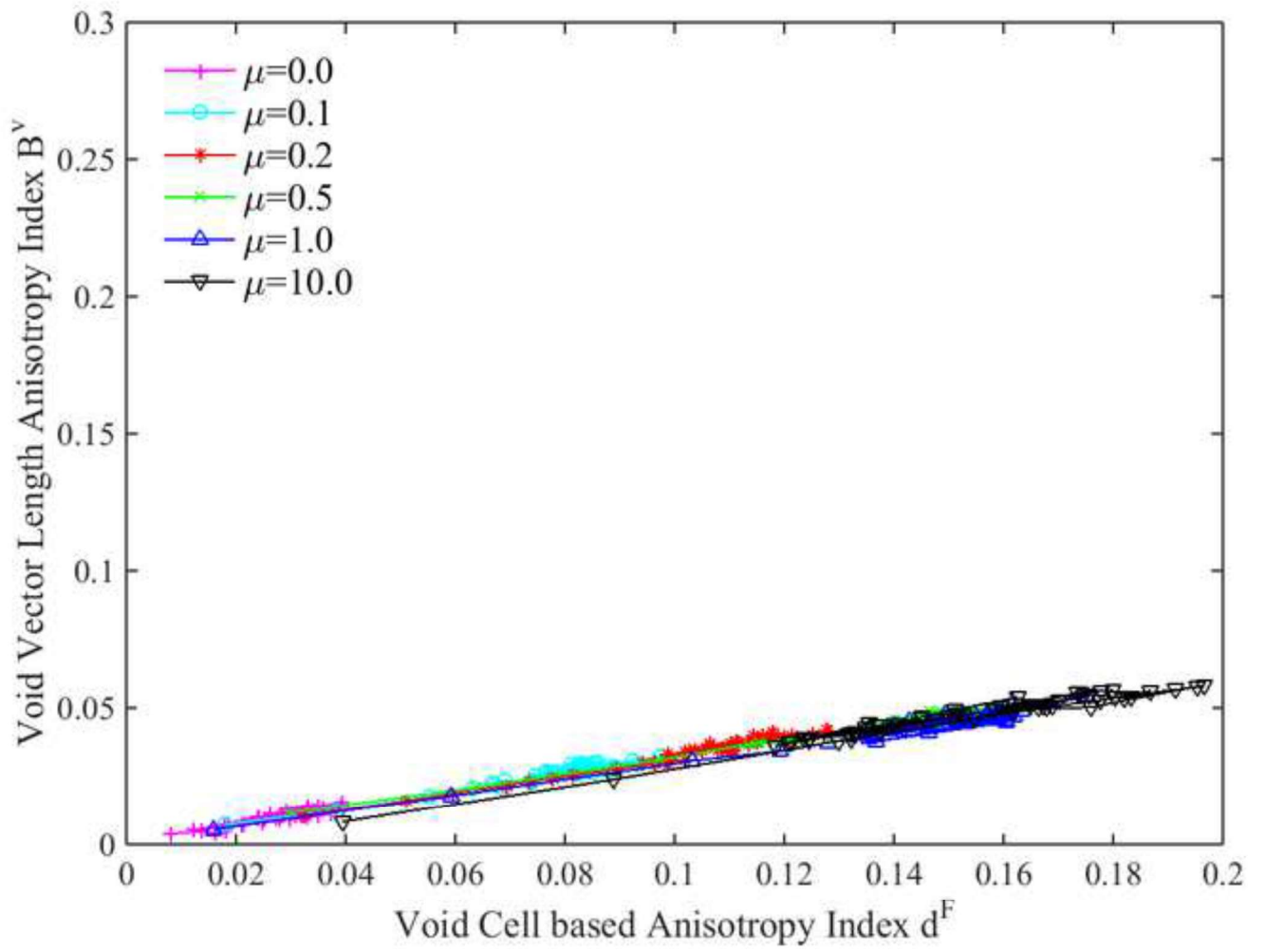






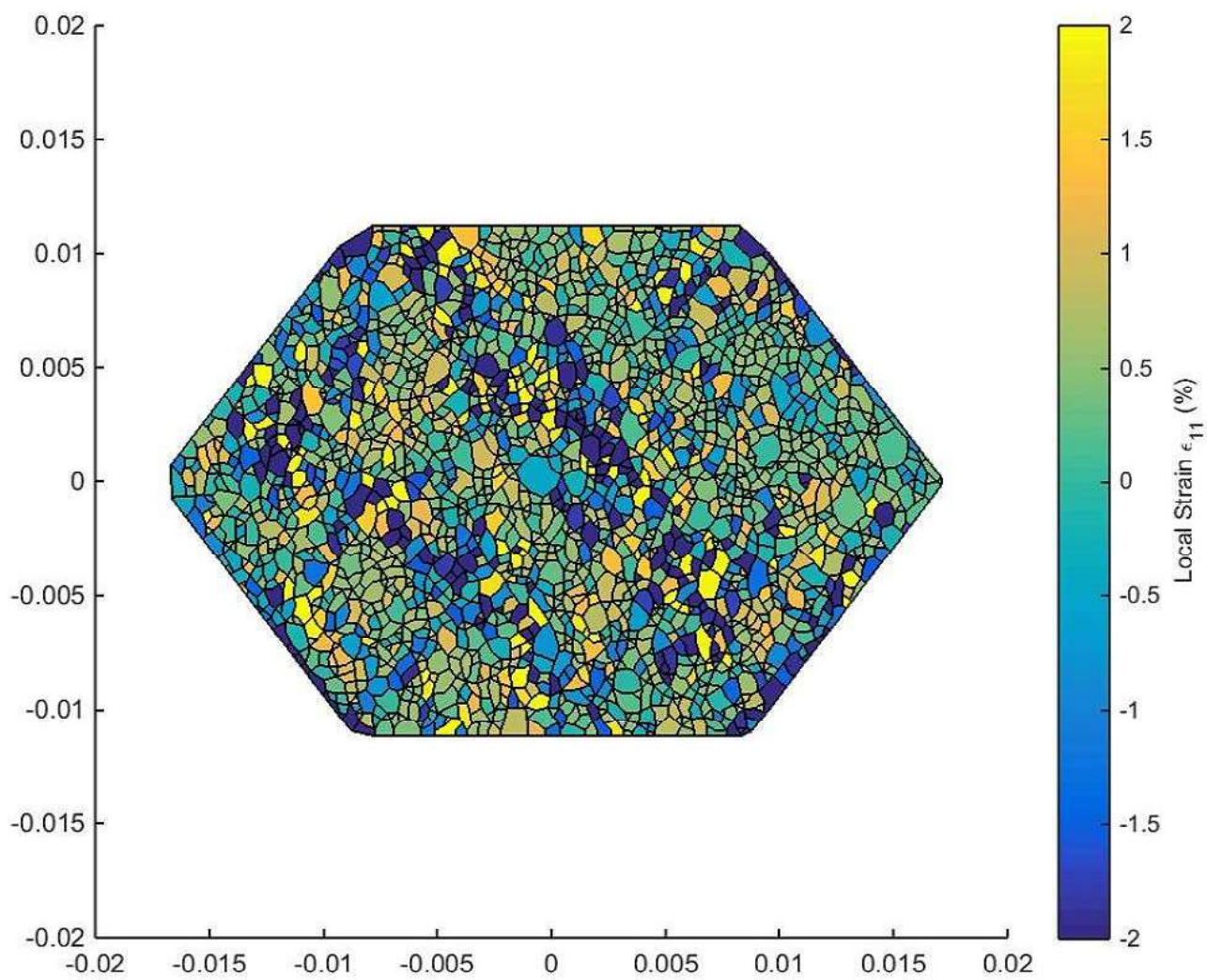






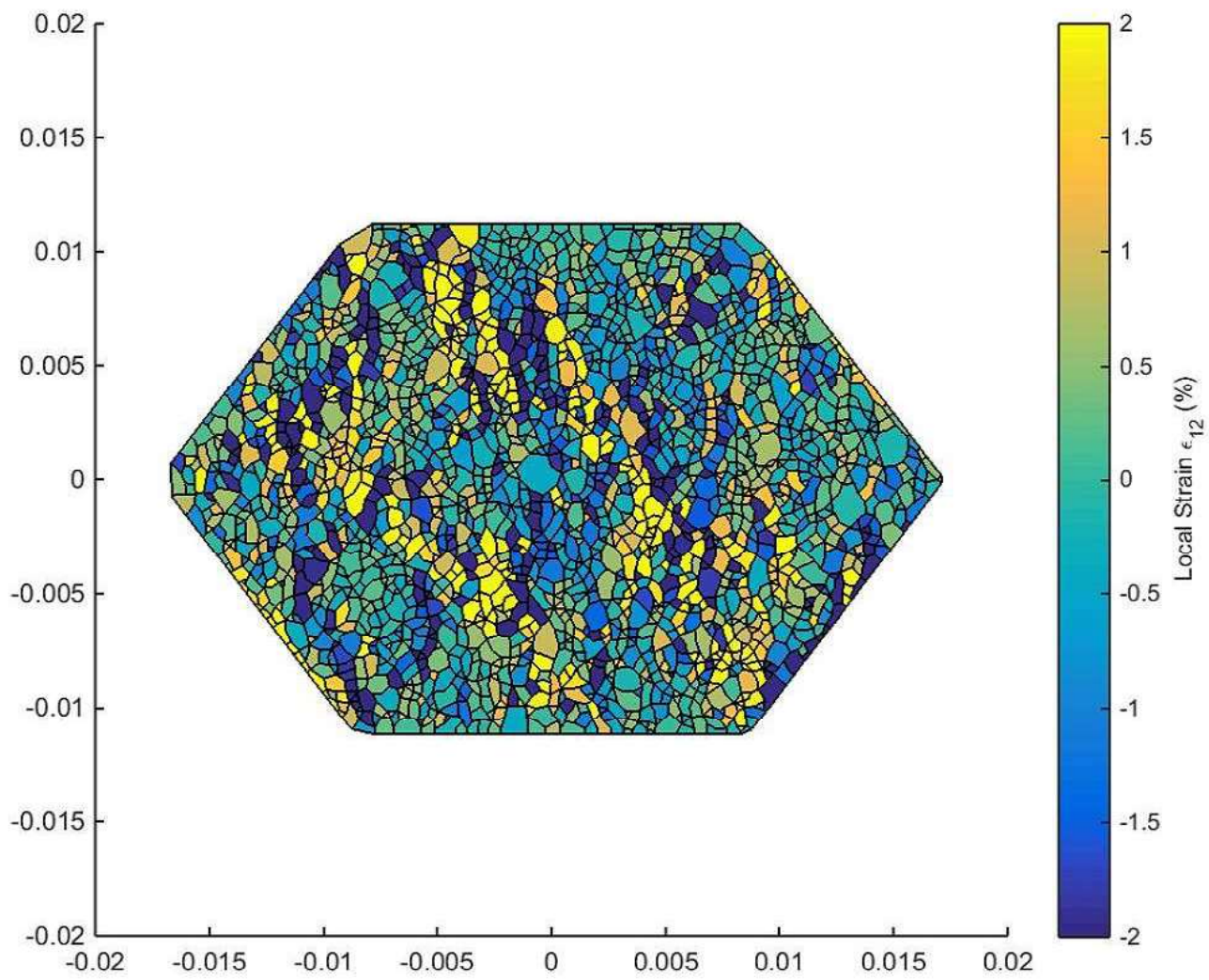
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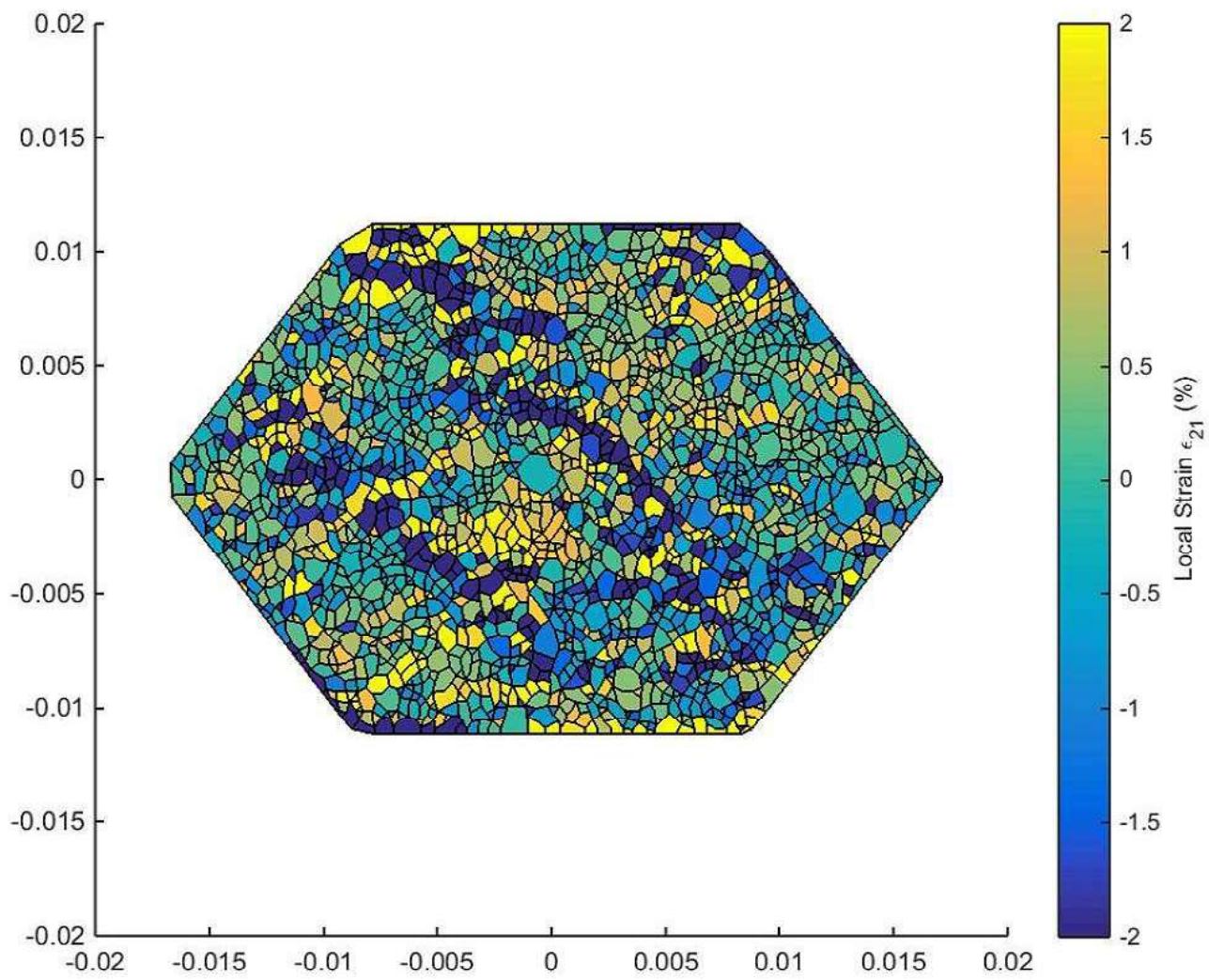
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