Effects of polydispersity on the micro-macro behavior of granular assemblies under different deformation paths

N. Kumar, O. I. Imole, V. Magnanimo and S. Luding

Multi Scale Mechanics (MSM), Faculty of Engineering Technology, MESA+,
University of Twente, P.O. Box 217, 7500 AE Enschede, The Netherlands
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Abstract

The micromechanical and macromechanical behavior of idealized granular assemblies, made by linearly elastic, frictionless, polydisperse spheres, are studied in a periodic, triaxial box geometry, using the discrete element method. Emphasis is put on the effect of polydispersity under purely isotropic loading and unloading, deviatoric (volume conserving) pure shear, and uniaxial compression paths.

We show that scaled pressure, coordination number and fraction of rattlers, behave in a very similar fashion as functions of volume fraction, irrespective of the deformation path applied. Interestingly, they show a systematic dependence on the deformation mode and polydispersity via the respective jamming volume fraction. This confirms that the concept of a single jamming point has to be rephrased to a "wide range" of values, dependent on microstructure and history of the sample.

This behavior is confirmed when a simplified constitutive model involving structural anisotropy is calibrated using the deviatoric simulations as the basic model parameters are found to depend on the polydispersity of the sample through the jamming volume fraction.The predictive power of the calibrated model is confirmed by comparison with an independent test, namely the uniaxial compression. The important features of the uniaxial experiment are captured and a qualitative prediction for the evolution of stress and fabric is shown involving a "softening" regime in both stress and fabric – stronger for the latter – that was not prescribed into the model a-priori.

Keywords: Polydispersity, Anisotropy, deformations, calibration, PARDEM.

1 Introduction and Background

Granular materials are widely used as raw materials in various industrial applications, including pharmaceutical, mining, chemical, agricultural, household products and food sectors. Processes involving milling, segregation, fragmentation, agglomeration, filtration and sieving, among others are common and often lead to the generation of granular systems with large size ratios. The optimization of these systems are exceptionally challenging and often require heuristic assumptions to be made. It is known, however that polydispersity influences the micro-mechanical behavior of granular systems. For example, the shear strength and packing fraction, which are important quantities in determining the stress state and response of granular assemblies have been shown to be influenced by the size ratio of the packing (Göncü & Luding, 2013; Shaebani et al., 2012).

On the other hand, the bulk macroscopic behavior of granular systems originates from the contact force network between their constituent particles. The contact force networks, even for systems with uniform size distribution, are mostly inhomogeneous leading to many interesting phenomena (Shaebani et al., 2012). In recent studies involving the effects of polydispersity, emphasis has been placed on systems with narrow size distributions – ostensibly to limit the effects of long-range structural order – with the exception of a few cases where wider distributions have been reported (Dodds & Weitz, 2002; Ogarko & Luding, 2012; Voivret et al., 2007, 2009). Additionally, a micromechanical description, which takes into account the discrete nature of granular systems, is necessary and must be linked to the continuum description, which involves the formulation of constitutive relations – for macroscopic fields. In recent

years, several constitutive relations have been proposed in literature (Goddard, 1998, 2010; Kolymbas et al., 1995; Mašín, 2012; Sun & Sundaresan, 2011; Thornton & Zhang, 2010), but only few take into account the anisotropy that develops when granular systems are subjected to shear deformation (Luding & Perdahcıoğlu, 2011; Magnanimo & Luding, 2011; Peyneau & Roux, 2008; Tejchman & Wu, 2007) and no study, to our knowledge connects anisotropy and polydispersity.

When a granular assembly is subjected to shear deformation, a buildup of shear stress is observed, along with an evolution of the structural anisotropy, which describes the creation and destruction of contacts (Ai et al., 2013; Alonso-Marroquin et al., 2005; Azéma & Radjaï, 2012; Hareb & Doanh, 2012; Kumar et al., 2013; Peyneau & Roux, 2008; Radjaï et al., 1999; Schröder-Turk et al., 2010; Walsh & Tordesillas, 2004). In this sense, anisotropy represents a history-parameter for the granular assembly. For anisotropic samples, scalar quantities are not sufficient to fully represent the internal direction dependent contact structure; therefore an extra tensorial quantity has to be introduced, namely the fabric tensor (Oda, 1972; Satake, 1982). To gain more insight into the microstructure of granular materials, numerical studies and simulations on various deformation experiments can be performed, see Hanley et al. (2012); Peyneau & Roux (2008); Thornton (2010); Thornton & Zhang (2006, 2010), among others.

In this study, we perform parametric studies with the goal of understanding the effect of polydispersity on both microscopic and macroscopic behavior of granular assemblies under isotropic, uniaxial and deviatoric deformation conditions. As (scalar and tensorial) microscopic quantities, we investigate the effects of polydispersity on coordination number, fraction of rattlers and fabric. The volumetric part of fabric is the measure of the strength of contact network, while the deviatoric part gives insight on the orientation of the contact network.On the macroscopic side, we consider the effects of polydispersity on the scaled pressure and the deviatoric stress. Another goal is to calibrate a constitutive model using parameters from deviatoric volume conserving pure shear simulations and test the predictive power of the calibrated model on an independent test, namely uniaxial compression test. We propose an objective definition for deviatoric stress and deviatoric fabric in a triaxial box and present findings on their behavior as a function of deviatoric strain. The parameters obtained from pure isotropic and deviatoric deformations are inserted into a constitutive model to predict uniaxial deformation.

This paper is organized as follows: The simulation method and parameters used and the generalized averaging definitions for scalar and tensorial quantities are given in section 2. The preparation and test procedures are explained in section 3. Polydispersity is introduced in subsection 4.1 and its effect on the evolution of the non-scaled pressure, coordination number and fraction of rattlers for the different deformation modes is discussed in subsection 4.2. In subsection 4.3, the macroscopic quantities (deviatoric stress and deviatoric fabric) and their evolution are studied as functions of polydispersity, volume fraction and deviatoric (shear) strain for the different deformation modes. Finally, these results are used to obtain/calibrate the macroscopic model parameters. Section 5 is devoted to theory, where we relate the evolution of the fabric anisotropy to that of stress and strain, as proposed in Luding & Perdahcıoğlu (2011); Magnanimo & Luding (2011), to display the predictive quality of the calibrated model.

2 Numerical simulation

The Discrete Element Method (DEM) (Cundall & Strack, 1979) has been used extensively in performing simulations in biaxial and triaxial geometries (Durán et al., 2010; Kruyt et al., 2010; Luding, 2005b; Sun & Sundaresan, 2011) involving advanced contact models for fine powders (Luding, 2008; Tomas, 2001), or general deformation paths, see Alonso-Marroquin et al. (2005); Thornton (2010); Thornton & Zhang (2010) and references therein. In this work, however, we restrict ourselves to the simplest deformation tests – namely isotropic, uniaxial and deviatoric –and to the linear contact model without friction. Since DEM is a standard method, only the contact model parameters relevant for our simulation are briefly discussed as well as the basic system parameters.

The simplest normal contact force model, which takes into account excluded volume and dissipation, linear repulsive and linear dissipative forces, is given as $\mathbf{f}_n = f_n\hat{\mathbf{n}} = (k\delta + \gamma\dot{\delta})\hat{\mathbf{n}}$, where k is the spring stiffness, γ is the contact viscosity parameter, δ is the overlap and $\dot{\delta}$ is the relative velocity in the normal direction $\hat{\mathbf{n}}$. An artificial background dissipation force, $\mathbf{f}_b = -\gamma_b\mathbf{v}_i$, proportional to the velocity $\mathbf{v}_i$ of particle i is added, resembling the damping due to a background medium, as e.g. a fluid. A short summary of the values of the parameters used in DEM simulations is shown in Table 1.[1] We waht to point out

[1]Note that the units are artificial and can be consistently rescaled to quantitatively match the values obtained from experiments (due to the simplicity of the contact model used), as shown in (Luding, 2008).

Parameter	Symbol	Value	S.I. Units
Time Unit	t_u	1	1 μs
Length Unit	l_u	1	1 mm
Mass Unit	m_u	1	1 μg
Number of Particles	N	9261	[–]
Average radius	$\langle r \rangle$	1	1 mm
Polydispersity	$w = r_{\max}/r_{\min}$	varied [1 – 10]	[–]
Particle density	ρ	2000	2000 [kg/m^3]
Normal stiffness	k	10^5	10^8 [kg/s^2]
Normal Viscosity	γ	1000	1 [kg/s]
Background viscosity	γ_b	100	0.1 [kg/s]

Table 1: Summary and numerical values of particle parameters used in the DEM simulations.

here that the choice of contact model (linear or non-linear) affects the collisional behavior between two particles as well as the bulk behavior (Ji & Shen, 2006; Shäfer et al., 1996). When linear and hertzian contact models are compared, a major difference is related to the initial contact stiffness, where the former presents a finite constant value, while for the later, the stiffness is a function of the deformation, namely it is zero at the beginning. However, the difference between the two models become smaller when the consolidation pressure becomes higher, as is the case in this study.

2.1 Microscopic Variables

In order to link the macroscopic load carried by the sample with the active microscopic contact network, all particles that do not contribute to the force network are excluded from the computation. Frictionless particles with less than 4 contacts are thus 'rattlers', since they cannot be mechanically stable and hence do not contribute to the contact network (Göncü et al., 2010; Imole et al., 2013; Madadi et al., 2004). The simple definition of coordination number is $C = M/N$, where M is the total number of contacts and $N = 9261$ is the total number of particles. If the overlap at a contact between two particles is greater than or equal to zero, i.e., $\delta \geq 0$, the contact contribute to the force network. The corrected coordination number is $C^* = M_4/N_4$, where, M_4 is the total number of contacts of the N_4 particles with at least 4 contacts, and the rattler fraction is $\phi_r = (N - N_4)/N$.

The total volume of particles is $\sum_{\mathcal{P}=1}^{N} V_{\mathcal{P}} = 4\pi N \langle r^3 \rangle/3$, where $\langle r^3 \rangle/3$ is the third moment of the size distribution discussed in detail in subsection 4.1 and the volume fraction is defined as $\nu = (1/V) \sum_{\mathcal{P}=1}^{N} V_{\mathcal{P}}$, where V is the volume of the box. Note that for the calculation of the total volume of particles, the volume which should be subtracted due to particle overlaps is neglected.

2.2 Macroscopic variables

Here, we focus on defining averaged macroscopic tensorial quantities – including strain-, stress- and fabric (structure) tensors – that reveal interesting bulk features and provide information about the state of the packing due to its deformation.

For any deformation, we can describe the external applied strain through the infinitessimal strain tensor $\mathbf{E}$. Its isotropic part ϵ_{v} (Göncü et al., 2010; Imole et al., 2013) is defined as:

$$\epsilon_{\mathrm{v}} = \dot{\epsilon}_{\mathrm{v}} \mathrm{d}t = \frac{\epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz}}{3} = \frac{1}{3}\mathrm{tr}(\mathbf{E}) = \frac{1}{3}\mathrm{tr}(\dot{\mathbf{E}})\mathrm{d}t, \tag{1}$$

where $\epsilon_{\alpha\alpha} = \dot{\epsilon}_{\alpha\alpha}\mathrm{d}t$ with $\alpha\alpha = xx$, yy and zz as the diagonal elements of $\mathbf{E}$ in the Cartesian x, y, z reference system. The trace integral of $3\epsilon_{\mathrm{v}}$, denoted as the volumetric strain ε_v is the true or logarithmic strain, i.e., the volume change of the system relative to the initial reference volume, V_0.

From the DEM simulations, one can determine the stress tensor as

$$\boldsymbol{\sigma} = (1/V) \sum_{c \in V} \mathbf{l}^c \otimes \mathbf{f}^c, \tag{2}$$

which is an average over the contacts in the volume V of the dyadic products between the branch vector $\mathbf{l}^c$ and the contact force $\mathbf{f}^c$, where the contribution of the kinetic energy has been neglected (Imole et al., 2013; Luding, 2005a). The isotropic component of the stress is the pressure $P = \mathrm{tr}(\boldsymbol{\sigma})/3$.

Besides the stress, we will focus on the fabric tensor in order to characterize the geometry/structure of the static aggregate, defined as

$$\mathbf{F} = (1/V) \sum_{\mathcal{P} \in V} V^{\mathcal{P}} \sum_{c \in \mathcal{P}} \mathbf{n}^c \otimes \mathbf{n}^c, \tag{3}$$

where $V^{\mathcal{P}}$ is the particle volume for particle $\mathcal{P}$, which lies inside the averaging volume V, and $\mathbf{n}^c$ is the normal unit branch-vector pointing from center of particle $\mathcal{P}$ to contact c (Kumar et al., 2013; Luding, 2005a). The average isotropic fabric is $F_{\mathrm{v}} = \mathrm{tr}(\mathbf{F}) = g_3 \nu C$, where ν and C are, respectively, the volume fraction, the coordination number, and g_3 is a function of moments of the size distribution (Göncü et al., 2010; Shaebani et al., 2012), as explained in detail in subsection 4.1. We want to highlight here that a different formulation for the fabric tensor considers simply the average orientation of contacts as follows (La Ragione & Magnanimo, 2012; Oda, 1972; Satake, 1982):

$$\mathbf{F}^s = \frac{1}{N_c} \sum_{c \in N_c} \mathbf{n}^c \otimes \mathbf{n}^c \,, \tag{4}$$

where N_c is the total number of contacts. The relationship between Eq. (3) and Eq. (4) is:

$$\mathbf{F}^s = \frac{\mathbf{F}}{g_3 \nu C} = \frac{3\mathbf{F}}{F_{\mathrm{v}}}. \tag{5}$$

In addition to the isotropic components, we use the following definition to quantify the magnitude of the deviatoric parts (Kumar et al., 2013) of tensors $\mathbf{Q}$ (stress $\boldsymbol{\sigma}$, strain $\mathbf{E}$ or fabric $\mathbf{F}$) :

$$Q_{\mathrm{dev}} = \mathrm{Fsgn}\left(\mathbf{Q}\right) \sqrt{\frac{\left(Q_{xx} - Q_{yy}\right)^2 + \left(Q_{yy} - Q_{zz}\right)^2 + \left(Q_{zz} - Q_{xx}\right)^2 + 6\left(Q_{xy}^2 + Q_{yz}^2 + Q_{zx}^2\right)}{2}}, \tag{6}$$

where Q_{xx}, Q_{yy} and Q_{zz} are the diagonal components, and Q_{xy}, Q_{yz} and Q_{zx} are the off-diagonal components of the symmetric tensor $\mathbf{Q}$. $\mathrm{Fsgn}\left(\mathbf{Q}\right)$ is the sign function with possible values as $+1$, 0 and -1, whose definition depends on the deformation path (see section 4.3). In the case of stress, Eq. (6) equals von Mises stress, $\sigma_{\mathrm{dev}} = \sqrt{3J_2}$, with J_2 as the second deviatoric stress invariant J_2.

When a biaxial or triaxial compression is performed, such that the strain, stress and fabric stay almost coaxial with principal axes parallel to the initial reference system, the off-diagonal terms become negligible and the diagonal terms coincide with the eigenvalues.

3 Preparation and test procedure

After the (common) initial isotropic preparation, the packing is deformed following three different procedures, namely isotropic, uniaxial and deviatoric paths (a detailed procedure can be found in (Imole et al., 2013)). For convenience, the definitions of the different modes will be based on their respective strain-rate tensors. Also note that the deformations applied to systems are always 'slow' enough to maintain the quasi-static regime and hence minimize the dynamical effects (Hanley et al., 2012; Imole et al., 2013).

3.1 Initial Isotropic preparation

Since careful, well-defined sample preparation is essential in any physical experiment to obtain reproducible results, the preparation consists of three parts: (i) randomization, (ii) isotropic compression, and (iii) relaxation, all equally important to achieve the initial configurations for the following analysis. (i) The initial configuration is such that spherical particles are randomly generated in a 3D box without

gravity, with low volume fraction and rather large random velocities, such that they have sufficient space and time to exchange places and to randomize themselves. (ii) This granular gas is then isotropically compressed, in order to approach a direction independent initial configuration with target volume fraction $\nu_0 = 0.64$, sightly below the jamming volume fraction, i.e. the transition point from fluid-like behavior to solid-like behavior (Majmudar et al., 2007; Makse et al., 2000; O'Hern et al., 2002; van Hecke, 2009). (iii) This is followed by a relaxation period at constant volume fraction to allow the particles to fully dissipate their energy and to achieve a static configuration in mechanical equilibrium, after sufficient relaxation indicated by the drop in kinetic to potential energy ratio to almost zero.

3.2 Isotropic compression mode

Further isotropic compression (negative strain-rate in our convention) can now be used to prepare initial configurations at different volume fractions, each one with subsequent relaxation, achieved at different steps during loading and unloading, as displayed in Fig. 1. Furthermore, this path can be considered as the isotropic element test by itself (Göncü et al., 2010). It is realized by a simultaneous inward movement of all the periodic boundaries of the system, with diagonal strain rate tensor

$$\dot{\mathbf{E}} = \dot{\epsilon}_{\mathrm{v}} \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix},$$

where $\dot{\epsilon}_{\mathrm{v}}$ (> 0) is the rate amplitude applied to the walls until the target maximum volume fraction $\nu_{\max} = 0.82$ is achieved. The simulations are continued with negative $\dot{\epsilon}_{\mathrm{v}}$ in the unloading mode, until the initial ν_0 is reached. The unloading branch configurations are more reliable since this part of the deformation is much less sensitive to the protocol and rate of deformation during preparation (Göncü et al., 2010; Imole et al., 2013) – that is we will use those initial states for our analysis.

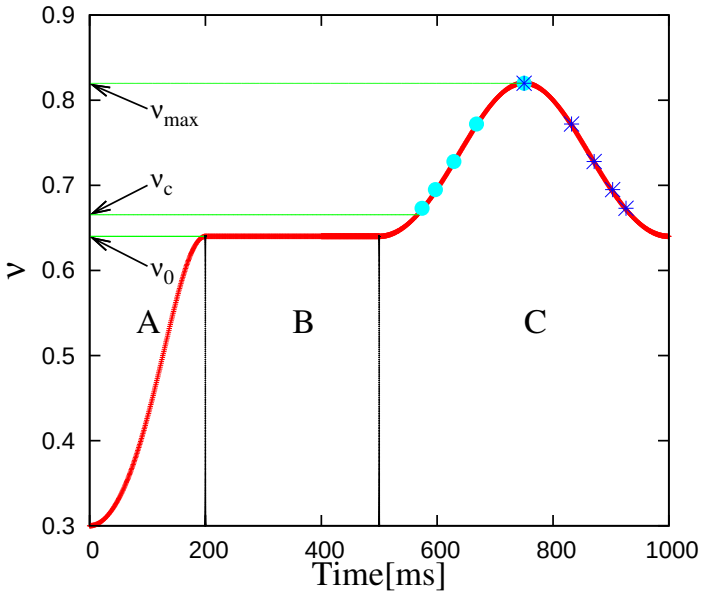


Figure 1: Evolution of volume fraction as a function of time. Region A represents the initial isotropic compression below the jamming volume fraction. B represents relaxation of the system to fully dissipate the systems energy and C represents the subsequent isotropic compression up to $\nu_{\max} = 0.820$ and then decompression. Cyan dots represent some of the initial configurations, at different ν_i, during the loading cycle and blue stars during the unloading cycle, at the same ν_i, which can be chosen for further study.

3.3 Uniaxial compression mode

Uniaxial compression is one of the element tests that is initiated at the end of the "preparation". The uniaxial compression mode in the triaxial box is achieved by a prescribed strain path in the z-direction,

while the other boundaries x and y are non-mobile. During loading (compression) the volume fraction increases, like for isotropic compression, from $\nu_0 = 0.64$ to a maximum volume fraction of $\nu_{\max} = 0.820$ (as shown in region C of Fig. 1), and reverses back to the original volume fraction ν_0 during unloading. Uniaxial compression is defined by the strain-rate tensor

$$\dot{\mathbf{E}} = \dot{\epsilon}_{\mathrm{u}} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix},$$

where $\dot{\epsilon}_{\mathrm{u}}$ is the strain-rate (compression > 0 and decompression/tension < 0) amplitude applied. The negative sign (convention) of $\dot{E}_{zz}$ corresponds to a reduction of length, so that tensile deformation is positive. Even though the strain is imposed only on the mobile "wall" in the z-direction, which leads to an increase of compressive stress on this wall during compression, also the non-mobile walls experience some stress increase due to the "push-back" stress transfer and rearrangement of the particles during loading, as discussed in more detail in the following sections. This is in agreement with theoretical expectations for solid materials with non-zero Poisson ratio. However, the stress on the passive walls is typically smaller than that of the mobile, active wall, as consistent with findings from laboratory element tests using the biaxial tester (Morgeneyer & Schwedes, 2003; Zetzener & Schwedes, 1998) or the so-called λ-meter (Kwade et al., 1994a,b).

3.4 Deviatoric deformation mode

The preparation procedure, as described in subsection 3.1, provides different initial configurations with volume fractions ν_i. Starting from the values ν_i in the unloading branch of isotropic configurations as shown in Fig.1, we perform volume conserving deviatoric deformations with the strain-rate tensor

$$\dot{\mathbf{E}} = \dot{\epsilon}_{\mathrm{D2}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix},$$

where $\dot{\epsilon}_{\mathrm{D2}}$ is the strain-rate (compression > 0) amplitude applied to the wall with normal in z-direction. The chosen deviatoric path is on the one hand similar to the pure-shear situation[2], and on the other hand allows for simulation of the biaxial experiment (with two walls static, while four walls are moving (Morgeneyer & Schwedes, 2003; Zetzener & Schwedes, 1998)), in contrast to the more difficult isotropic compression, where all the six walls are moving. Different types of volume conserving deviatoric deformations can be applied to shear the system, but very similar behavior has been observed (Imole et al., 2013).

4 Polydispersity

Most granular materials are highly polydisperse in nature. It is known that size polydispersity affects the mechanical behavior of granular systems (e.g., shear strength) as well as their space-filling properties (e.g., packing fraction) (Göncü & Luding, 2013; Ogarko & Luding, 2012), which are crucial in many engineering applications like road construction or soils liquefaction problems (see (Anderson, 1996; Belkhatir et al., 2012, 2011) and references therein). Nevertheless the attention has been restricted so far to monodisperse or binary mixtures or narrow size distribution. Here we use samples with different degrees of polydispersity to study the effect of increasing polydispersity on the evolution of microscopic and macroscopic parameters during various deformation modes.

4.1 Polydispersity

We define polydispersity in terms of the width $w = r_{\max}/r_{\min}$ – where $r_{\max}$ and $r_{\min}$ represent the radius of the largest and smallest particles in the overall ensemble of a distribution uniform in size (Göncü et al.,

[2]Pure shear is here used to identify constant volume deviatoric loading with principal strain axis keeping the same orientation as the geometry (cubical) of the system for the whole experiment. In this case, there is no rotation (vorticity) of the strain principal axis and no distortion/rotation of the sample due to deformation.

2010; Göncü & Luding, 2013):

$$f(r) = \frac{w+1}{2(w-1)\langle r\rangle}\Theta\left(\frac{2w\langle r\rangle}{w+1} - r\right)\Theta\left(r - \frac{2\langle r\rangle}{w+1}\right), \tag{7}$$

with step function $\Theta(x \geq 0) = 1$ and $\Theta(x < 0) = 0$. From the distribution of radius, one can calculate the parameter g_3 that describes the polydispersity of a 3D spherical system, (Göncü et al., 2010) as:

$$g_3 \approx \frac{1 - B_2 + C_2 + (B_2 - 2C_2)\dfrac{\langle r^4\rangle}{\langle r\rangle\langle r^3\rangle} + C_2\dfrac{\langle r^5\rangle}{\langle r\rangle^2\langle r^3\rangle}}{1 + C_2\left[\dfrac{\langle r^2\rangle}{\langle r\rangle^2} - 1\right]}, \tag{8}$$

where the constants $B_2 = 1.077$ and $C_2 = 0.2629$ are described in (Göncü et al., 2010) and $\langle r^n\rangle$ is the n^{th} moment of r up to the 5^{th} degree. Only for the monodisperse case, the simplification $g_3 = 1$ holds. Otherwise, it increases with polydispersity w and saturates at high values about 1.627.

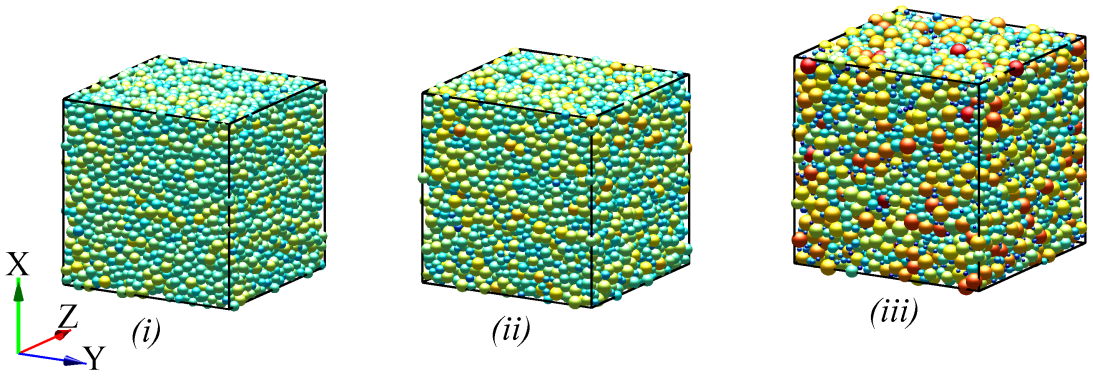


Figure 2: Snapshots of three systems with polydispersity (i) 1.5, (ii) 2 and (iii) 5 respectively with the same volume fraction $\nu = 0.82$. The color code indicates the contacts of the particles : (red: big contacts, blue: no contacts).

In order to study the effect of polydispersity on micro-macro behavior of granular assembly, we prepare different packings with polydispersity ranging from $w = 1$ to 10. These packings are deformed following the paths described in section 3. As an example, we show in Fig. 2 isotropic samples with $w = 1.5$, 2 and 5 for constant volume fraction $\nu = 0.82$. Note that for the same volume fraction ν, the volume of the box is higher for higher polydispersity, since $\langle r^3\rangle$ increases with w for fixed $\langle r\rangle = 1$. For higher polydispersity, particles of smaller size fill more efficiently the pore space between larger particles. However, lower polydispersity in packings of granular materials is associated with alterations in the structural order (Ogarko & Luding, 2012; Voivret et al., 2007). [3]

4.2 Effect of polydispersity on isotropic quantities

In the following, we will study the influence of polydispersity on scaled pressure, coordination number and fraction of rattlers, during the three deformation paths described above.

4.2.1 Confining pressure

Starting from Eq. (2), we define the non-dimensional pressure (Göncü et al., 2010; Imole et al., 2013) as

$$p = \frac{2\langle r\rangle}{3k}\mathrm{tr}\,(\boldsymbol{\sigma})\,, \tag{9}$$

with $\langle r\rangle$ the first radius moment (average radius) and k the spring stiffness defined in section 2, while the scaled pressure is:

$$p^* = \frac{p\nu_c}{\nu C} = p_0(-\varepsilon_{\mathrm{v}})\left[1 - \gamma_p(-\varepsilon_{\mathrm{v}})\right] \tag{10}$$

[3]Note that here results for a uniform radius distribution are presented. The trend will be different if the type of distribution is different e.g., uniform surface or uniform volume distribution.

where p_0, γ_p, and the critical volume fraction ν_c are fit parameters. When comparing the two expressions of non-dimensional and scaled pressure, we notice that in Eq. (10), the pressure is normalized by "νC", that is the contribution of the density of contacts and is cancelled and p^* is then only proportional to the average deformation (overlap) of the particles at a given volume fraction and to the distance from jamming point through ν_c.

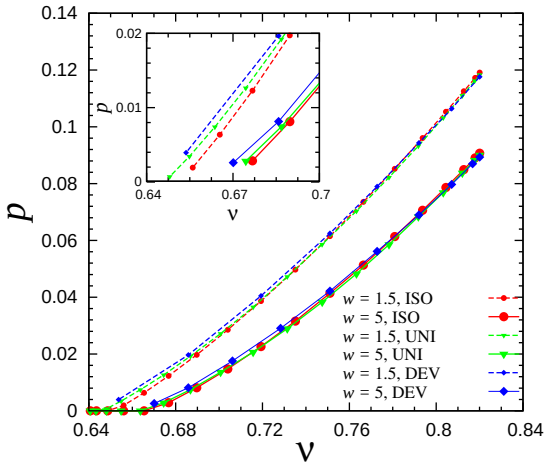


Figure 3: Evolution of non-dimensional pressure p with volume fraction ν for the isotropic (●, red), uniaxial (▼, green) and deviatoric (◆, blue) deformation modes, as shown in the legend. Small symbols represent $w = 1.5$ and big symbols represent $w = 5$. Inset is the zoomed-in area near the jamming volume fraction.

In Fig. 3, we plot the evolution of the non-dimensional pressure p with volume fraction ν during isotropic, uniaxial and deviatoric deformation for polydispersities $w = 1.5$ and 5. Note that p increases with ν starting from ν_c, with slight differences related to different modes, as discussed in (Imole et al., 2013). For a given volume fraction, we observe a decrease in the pressure with increasing polydispersity. Better insights on this feature are given by looking at the the distribution of overlaps $\delta(r)/\langle r\rangle$ as a function of the scaled particle radii $r_{\rm sc}$, as shown in Figs. 4(a) and 4(b) for two volume fractions, $\nu = 0.686$ and $\nu = 0.82$. The particle radii are scaled such that $r_{\rm sc} = 0$ and $r_{\rm sc} = 1$ represent the smallest and largest particle in the configuration, respectively. A first observation is the unsurprising increase in the average overlap for all modes and polydispersities with increasing compression from $\nu = 0.686$ in Fig. 4(a) to $\nu = 0.82$ in Fig. 4(b), in agreement with Fig. 3. Based on this, we can claim that $P/k \propto \delta(r)/\langle r\rangle$, at least for small deformations and for linear contact model. In addition, for both volume fractions shown, the overlap increases with increasing particle radii.

Focusing on the deformation modes trend, for both polydispersities, deviatoric deformation leads to the highest pressure, followed by the uniaxial and isotropic modes, respectively. This trend is clearly visible at lower volume fractions – as shown in the inset of Fig. 3, while for increasing volume fraction, the effect of the deformation mode reduces, as evident by the collapse of data in Fig. 4(b). The agreement is confirmed by observing the average overlap $\langle\delta\rangle$ in Figs. 4(a) and 4(b), with the data from uniaxial compression lying between the isotropic and deviatoric datasets. The trend observed in the evolution of the scaled pressure and distribution of the average overlaps are consistent with the fact that the isotropic and deviatoric modes are pure modes, while the uniaxial mode is a superposition of isotropic and deviatoric modes (Luding & Perdahcıoğlu, 2011).

Figs. 5(a – c) show the effects of varying polydispersity on the scaled pressure in Eq. (10), where p^* is plotted against volumetric strain $-\varepsilon_v$ for isotropic, uniaxial and deviatoric deformations. For a single deviatoric deformation the volume fraction is constant during the path and hence the pressure remains practically constant. In this work the data describing deviatoric mode will always refer to the values in the critical state, after large deformation (see Imole et al. (2013) for more details), unless stated otherwise. In the small strain region, for all deformation modes, the datasets collapse on each other. Only with increasing $-\varepsilon_v$, a small deviation of the simulation data is observed for the isotropic and deviatoric modes, due to the non-linear correction that shows up at large strain in Eq. (10). The analytical expression of the scaled pressure in Eq. (10) fits the simulation data well for all three deformation modes and polydispersity, in agreement with findings in Göncü et al. (2010); Göncü & Luding (2013); Imole et al. (2013).

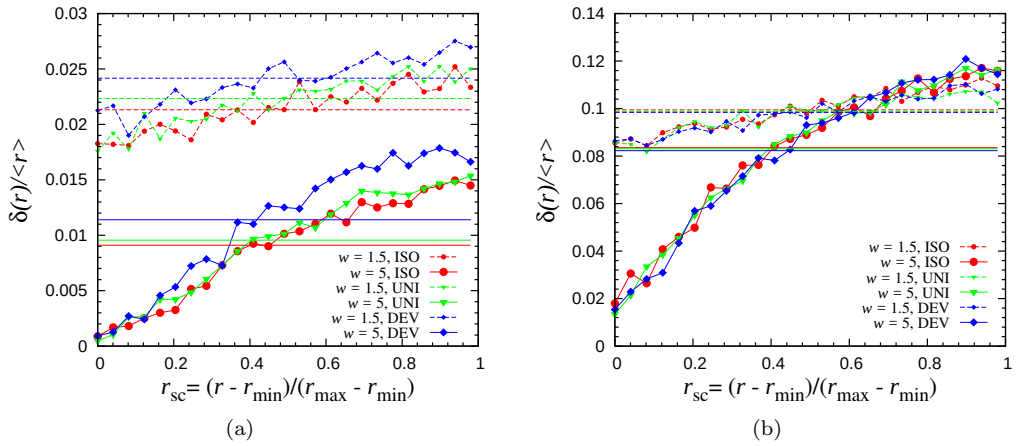


Figure 4: Average overlap δ per particle for a radius range scaled by average radius $\langle r \rangle$, plotted against a scaled radius axis $r_{\rm sc} = (r - r_{\rm min})/(r_{\rm max} - r_{\rm min})$ for the isotropic (•, red), uniaxial (▼, green) and deviatoric (♦, blue) deformation modes. Small symbols represent $w = 1.5$ and big symbols represent $w = 5$. Volume fractions are (a) $\nu = 0.686$ (b) $\nu = 0.82$. Solid and dashed horizontal lines are average overlap $\langle \delta \rangle$ in the system for the three modes for $w = 1.5$ and $w = 5$ respectively. Note that the y-axis range is different in the two plots.

Mode	ν_c^0	ν_c^∞
ISO	0.6710	0.6967
UNI	0.6675	0.6956
DEV	0.6647	0.6913
Ogarko & Luding (2012)	0.65	0.6828

Table 2: Summary of parameters ν_c^0 and ν_c^∞ using Eq. (11) presented in Fig. 7, for the isotropic, uniaxial and deviatoric deformation modes.

The comparison of Figs. (3) and (4) puts in evidence a very interesting feature in the behavior of pressure. When the contact density νC is scaled out in p^*, the curves collapse irrespective of polydispersity leading to the conclusion that this factor affects the contact network while the deformation mode (and the distance from jamming) influences the evolution of average overlap. The fit parameters for p^* in Eq. (10) are given in Fig. 6 (and Table 4 in the appendix). The parameter p_0 is fairly constant with increasing polydispersity, with p_0 values higher for the isotropic case and uniaxial and deviatoric p_0 being very close. This is in agreement with expectations, as in both uniaxial and deviatoric deformations, anisotropy develops along the path, and the value of the non-dimensional pressure is increasing with respect to the (pure) isotropic case. The non-linear contribution from γ_p fluctuates for smaller polydispersity and becomes significant for higher w.

From the analysis of the pressure behavior by fitting Eq. (10), we can extract the dependence of the jamming volume fraction ν_c on the polydispersity w and the deformation mode, as shown in Fig. 7. The jamming volume fraction increases with increasing polydispersity, with ν_c for the isotropic case giving highest values. The ν_c law for the 'mixed' uniaxial mode is bordered on both sides by the isotropic and deviatoric datasets. This is consistent with findings in Imole et al. (2013) where $\nu_c^{\rm ISO} > \nu_c^{\rm UNI} > \nu_c^{\rm DEV}$. In this case a similar argument holds as mentioned for p_0, related to developing anisotropy during the over-compression, that explains the trend of the jamming point between isotropic, deviatoric and uniaxial. This confirms that the jamming volume fraction is *not a single value* but depends on the deformation history of the packing.

A theoretical prediction for the variation in ν_c under isotropic compression of polydisperse hard spheres is presented by Ogarko & Luding (2012):

$$\nu_c(w) = \nu_c^\infty - \left(\nu_c^\infty - \nu_c^0\right)\left(3w^{-2} - 2w^{-3}\right), \tag{11}$$

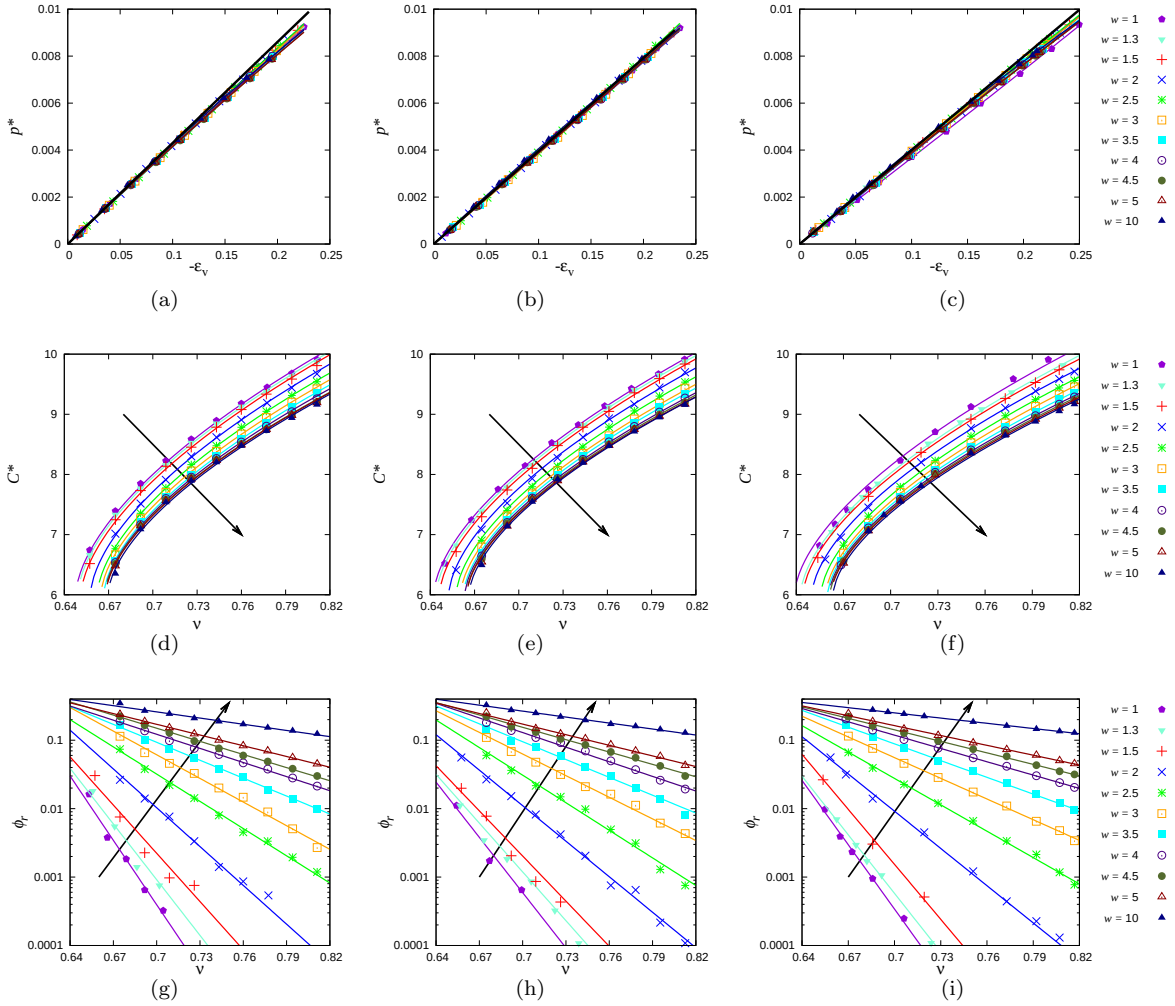


Figure 5: Effect of polydispersity w on scaled pressure p^*, coordination number C^*, and fraction of rattlers ϕ_r for the three deformation modes namely, isotropic compression (first column), uniaxial compression (middle column) and deviatoric deformation (right column). The solid lines are the fits to the corresponding macroscopic properties using Eqs. (10), (12) with $C_0 = 6$, $\alpha = 0.60$ for the three modes, and (13). The arrows indicate the increasing polydispersity. The solid black line in the p^* plot is Eq. (10) without the non-linear term. All the fit parameters are presented in Table 4 in the appendix.

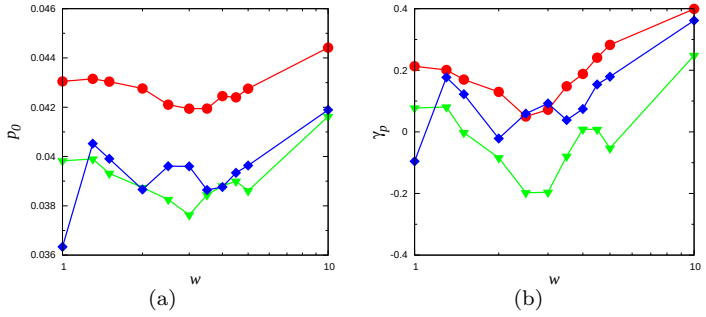


Figure 6: Comparison of the fit parameters (a) p_0 and (b) γ_p with polydispersity w for the analytical equations of scaled pressure p^* using Eq. (10) for the isotropic (•, red), uniaxial (▼, green) and deviatoric (⧫, blue) deformation modes. The fit parameters are presented in Table 4 in the appendix.

where ν_c^0 and ν_c^∞ are the jamming volume fractions for $w = 1$ and $w \to \infty$ respectively. We apply Eq.

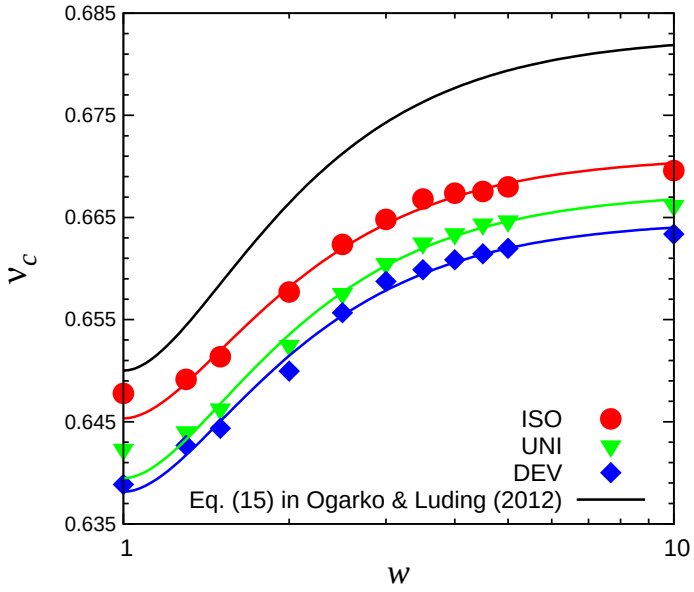


Figure 7: Evolution of jamming point ν_c with polydispersity w for the deformation modes considered. Corresponding solid lines are the theoretical predictions for different modes using Eq. (11). Note that the fit is applied only to $w > 1.2$, since local crystallization (Ogarko & Luding, 2012; Schröder-Turk et al., 2010) might happen at lower polydispersity causing ν_c values much higher than the disordered, random prediction.

(11) to the three deformation modes, and in Fig. 7 we show the prediction for hard spheres together with the ν_c simulation data for the three modes, and the fitting curves, where the parameters ν_c^0 and ν_c^∞ are presented in Table 2. Besides the quantitative disagreement due to the difference between hard and soft spheres, both systems show a very similar trend, the predictions working well for all the three modes. The simulations in Ogarko & Luding (2012), leading to Eq. (11), were carried out by very slow isotropic compression from the low density collisional regime, where the fluctuation velocities were not relaxed as done in this study. The strong kinetic energy fluctuations represent a type of 'tapping' that allows the system to relax to better packed configurations with larger ν_c. The data in Fig. 7 from Ogarko & Luding (2012) thus represents an upper limit of optimal compaction, which is not reached by e.g. slow over-compression to $\nu_{\max} = 0.82$. Eq. (11) can then capture the evolution of ν_c with polydispersity, irrespective of the deformation modes, when the fit parameters are properly defined. This interesting feature shows that ν_c acts as a state variable, able to describe the configuration of the assembly and thus represent its history, as also reflected by the overlaps in Fig. 4.

4.2.2 Coordination Number

It has been shown in Göncü et al. (2010); Imole et al. (2013) that under isotropic deformation, the corrected coordination number, C^* follows the power law:

$$C^*(\nu) = C_0 + C_1 \left(\frac{\nu}{\nu_c} - 1 \right)^\alpha , \tag{12}$$

where $C_0 = 6$ is the isostatic value in the frictionless case. α and C_1 are fit parameters, while we use ν_c from p^* extrapolation analysis as input value, leading to one less fit parameter for C^*. We observe a very small variation (3 %) of α with polydispersity and deformation modes (Imole et al., 2013) but for simplicity we set it to a fixed value of 0.60 in this work (Peyneau & Roux, 2008). Only C_1 is then the residual free fit parameter.

In Figs. 5(d – f), we compare the evolution of the corrected coordination number C^* as a function of volume fraction ν during isotropic, uniaxial and after deviatoric loading and show its dependence on polydispersity. The behavior is qualitatively similar for all the three deformation paths: contacts close and the coordination number increases with increasing volume fraction. Moreover, for the three modes,

configurations with lower polydispersity result in a higher number of contacts per particle. The data are well fitted by Eq. (12) with the fit parameter C_1 as function of w shown in Fig. 8(a). A systematic decrease in C_1 is observed with increasing polydispersity. The C_1 values of the 'mixed' uniaxial mode lie between the isotropic and deviatoric datasets.

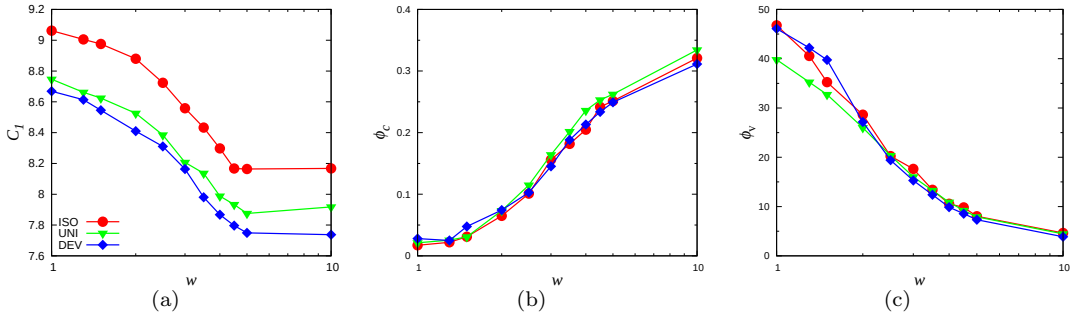


Figure 8: Comparison of the fit parameters for the analytical equations of coordination number C^* and rattler fraction ϕ_r using Eqs. (12) with $C_0 = 6$, $\alpha = 0.60$, and (13), respectively, for the isotropic (●, red), uniaxial (▼, green) and deviatoric (◆, blue) deformation modes. (a) Effect of polydispersity w on coordination number C^* fit parameters : C_1. (b – c) Effect of polydispersity w on rattler fraction ϕ_r fit parameters : ϕ_c and ϕ_v. The fit parameters are presented in Table 4 in the appendix.

Further increase in the polydispersity beyond $w = 4.5$ did not lead to a further change of C_1 – evidenced also by the collapse of the C^* lines on each other. This suggests that uniform size polydispersity influences the micromechanics only within a certain limit. For highly polydisperse packings ($w > 5$), the limit is approached because the critical volume fraction ν_c saturates (see Fig. 7).

In order to further investigate the behavior of the coordination number C^* we study the distribution of contacts per particle radius fraction. In Figs. 9(a) and 9(b), we plot the average number of contacts (excluding the rattlers) for a radius range, defined as $C^*(r)$, versus the scaled radius $r_{sc} = (r - r_{min})/(r_{max} - r_{min})$ for $\nu = 0.686$ and $\nu = 0.82$ for the three deformation modes. $C^*(r)$ increases with increasing r_{sc} for all the three modes, that is the number of contacts is bigger for bigger particles. This is expected because the bigger particles have larger surface area and thus can be in contact with more particles. A similar argument explains the relation between the particle coordination number $C^*(r)$ and polydispersity: smaller w leads to higher number of contacts for the smallest particles and to a weaker variation of $C^*(r)$ with r_{sc}. The crossover r_{sc} value shifts towards the left for higher volume fractions. As expected, for higher volume fractions, $C^*(r)$ increases faster with r_{sc}, as shown in Fig. 9(b), since more contacts are formed as the volume of the box becomes smaller. Comparing the deformation modes, only very minimal differences appear, visible for low volume fraction, $\nu = 0.686$, as shown in Fig. 9(a) and negligible for high volume fraction, $\nu = 0.82$, as seen in Fig. 9(b), in agreement with the argument proposed in Section 4.2.1 for p^*. The average values for isotropic deformation are smaller, larger for deviatoric, and the mixed uniaxial deformation mode lies in between the two (Imole et al., 2013).

4.2.3 Fraction of rattlers

The analytical expression for the fraction of rattlers is proposed in (Göncü et al., 2010; Imole et al., 2013) as

$$\phi_r(\nu) = \phi_c \exp\left[-\phi_v\left(\frac{\nu}{\nu_c} - 1\right)\right], \tag{13}$$

where ϕ_c and ϕ_v are fit parameters, and ν_c is the jamming volume fraction inferred from Eq. (10) for the different deformation modes. We show the effect of polydispersity on the fraction of rattlers under isotropic, uniaxial and deviatoric deformation in Figs. 5(g – i) and the fit parameters variation with w in Figs. 8(b) and 8(c) (numerical values are reported in Table 4 in the appendix). A first observation is that the fraction of rattlers decreases exponentially with increasing volume fraction (Imole et al., 2013) in agreement with Eq. (13). Furthermore, the increase of polydispersity leads to an increase of the fraction of rattlers in the system. This is not surprising since the volume occupied by finer/smaller particles is smaller in highly polydisperse systems. Contacts of these smaller particles are transient since they have

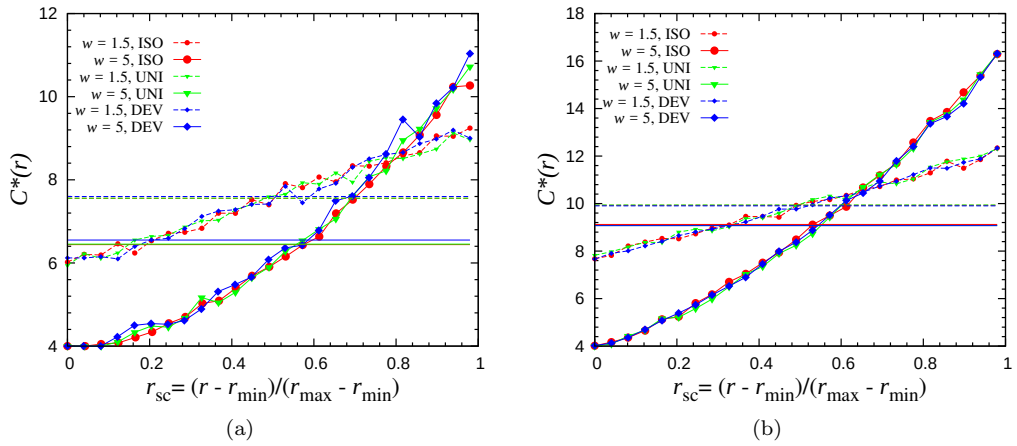


Figure 9: Average contacts per particle excluding the rattlers $C^*(r)$ for a radius range, plotted against a scaled radius $r_{\rm sc} = (r - r_{\rm min})/(r_{\rm max} - r_{\rm min})$ for the isotropic (•, red), uniaxial (▼, green) and deviatoric (♦, blue) deformation modes. Small symbols represent $w = 1.5$ and big symbols represent $w = 5$. Volume fractions are (a) $\nu = 0.686$, and (b) $\nu = 0.82$. Solid and dashed horizontal lines are the average coordination numbers $\langle C^*(r)\rangle = C^*$ in the system for the three modes, for $w = 1.5$ and $w = 5$ respectively. The y-axis range is different in the two plots.

more freedom to move within the system (for this size distribution – not in general). In some cases, they may become 'caged' between larger particles without having sufficient (four or more) contacts with their neighbors. This leads to a drop in the coordination number and an increase in the fraction of rattlers.

Also interesting is the evolution of the parameters of Eq. (13), ϕ_c and $\phi_{\rm v}$ which represents the initial point and the slope, respectively. A systematic increase in ϕ_c with increasing polydispersity is observed, whereas the slope $\phi_{\rm v}$ decreases with increasing polydispersity. This indicates that even though the fraction of rattlers in highly polydisperse systems is higher, the rate at which rattlers are lost in these systems during compression decreases with w. This again is related with the 'cage' argument, as very small particles are caged by big particles and need a high compression degree to gain new contacts with respect to medium sized particles (see Figs. 9(a) and 9(b)). Interestingly, both parameters ϕ_c and $\phi_{\rm v}$, as presented in Fig. 8, are seemingly unaffected by the deformation mode, stating that the history of the sample can be fully represented by ν_c, when the fraction of rattlers is analyzed.

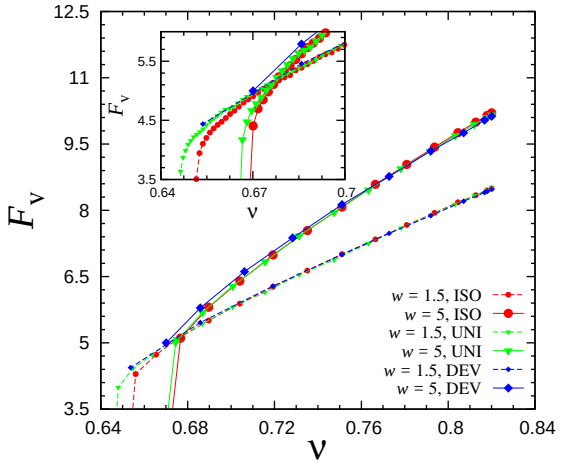


Figure 10: Evolution of isotropic fabric $F_{\rm v}$ with volume fraction ν for the isotropic (•, red), uniaxial (▼, green) and deviatoric (♦, blue) deformation modes as shown in the legend. Small symbols represent $w = 1.5$ and big symbols represent $w = 5$. Inset is the zoomed-in area near the jamming volume fractions.

Finally, we plot in Fig. 10 the evolution of the isotropic fabric $F_{\rm v} = g_3\nu C$ versus volume fraction during isotropic compression. $F_{\rm v}$ increases with volume fraction and polydispersity w and shows a trend

opposite with respect to the corrected coordination number C^* in Figs. 5(d – f). This can be explained by observing the rattlers: when particles with less than four contacts are included in the calculation of C, the values of F_v grow with increasing w and ν. For both polydispersities, near the jamming volume fraction, deviatoric deformation has the highest F_v, isotropic deformation has the lowest and the mixed uniaxial mode is in between the two – as shown in the inset of Fig. 10. This variations disappear for large volume fractions. However, the differences between the three modes for F_v are smaller compared to the isotropic part of stress p, as it is related to small differences in the average contact number per particle, as shown in Figs. 9(a) and 9(b).

4.3 Effect of polydispersity on deviatoric quantities

In this section, we present the effects of polydispersity on the evolution of deviatoric stress and deviatoric fabric during uniaxial and deviatoric deformation paths. The former, a macroscopic property quantifies the stress anisotropy (Imole et al., 2013), while the latter is a microscopic property related to the orientation of the contact network. Here, we focus on the simulation results for the uniaxial and deviatoric deformation modes (since the deviatoric quantities are only fluctuating around zero for the isotropic mode). Later in section 5, we will use the information obtained from the above mentioned quantities to calibrate a constitutive model. In the end, we will test the predictive power of the calibrated constitutive model on an independent uniaxial compression test.

4.3.1 Deviatoric stress

In Fig. 11(a), we plot the deviatoric stress ratio ($s_\mathrm{dev} = \sigma_\mathrm{dev}/P$) as a function of deviatoric strain ϵ_dev during deviatoric deformation for packings with three different polydispersities. The volume fraction ν is 0.751 in all cases, and stays constant during the numeric experiments. The deviatoric stress grows initially with rate β_s from random initial values (note the small random initial anisotropy present in each sample) until an asymptote, $s_\mathrm{dev}^\mathrm{max}$ at steady state is reached, where it remains fairly constant, in agreement with results in Cui & O'Sullivan (2006); Imole et al. (2013); Kumar et al. (2013); Luding (2004). The steady state value increases with polydispersity (the highly fluctuating values are in the range 0.11 ± 0.02, 0.12 ± 0.03 and 0.15 ± 0.035 for $w = 1.5, 2$ and 5, respectively). Surprisingly, while the deviatoric stress σ_dev is practically unaffected by w, the pressure P decreases with increasing polydispersity (see Fig. 3), leading to the dependence of the ratio σ_dev/P on w as observed. On the other hand, the slope β_s, proportional to the shear stiffness (scaled by pressure) of the initial isotropic configurations, is a function of the isotropic fabric F_v, as shown in the inset of Fig. 11(a). The relation between isotropic fabric and polydispersity, extensively discussed in (Göncü et al., 2010) and reported in Fig. 10, makes β_s a decreasing function of w.

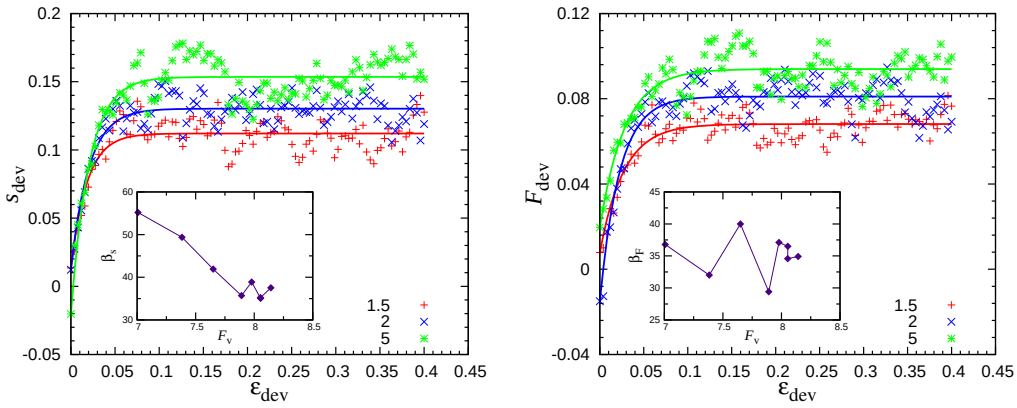
Furthermore, in Fig. 12(a) we plot the deviatoric stress as a function of deviatoric strain during uniaxial compression, for packings with different polydispersity $w = 1.5$, 2 and 5. The uniaxial test starts from initial volume fraction $\nu_i = 0.72$ (the same value used for the previous deviatoric simulations), and reaches the maximum volume fraction $\nu_\mathrm{max} = 0.82$. As for the deviatoric simulations, higher polydispersity leads to higher $s_\mathrm{dev}^\mathrm{max}$ at steady state also for the uniaxial deformations. The same argument about the dependence of pressure on polydispersity holds and explains the behavior in Fig. 12(a). We observe larger fluctuations for the uniaxial deformation mode with respect to the deviatoric one, with averages and errors $s_\mathrm{dev}^\mathrm{max} \approx 0.10 \pm 0.025$, 0.11 ± 0.035 and 0.15 ± 0.04 for $w = 1.5, 2$ and 5, respectively. We relate the increasing fluctuations to the non-conserved volume (Imole et al., 2013) and more "violent" rearrangements. Note that different sign conventions are used in Eq. (6) to calculate the deviatoric stress for deviatoric and uniaxial simulations, since the definition of the sign function Fsgn depends on the deformation mode, as discussed in section 2, i.e. the strain eigen-system. Since the latter is parallel to x, y, z, the sign function for uniaxial compression (negative strain components versus positive stress and fabric) is

$$\mathrm{Fsgn}\left(\mathbf{Q}\right) = \mathrm{sgn}\left(Q_{zz} - 0.5\left(Q_{xx} + Q_{yy}\right)\right),$$

where the z-wall is moving and the $x-$ and y-walls are not. For deviatoric deformation

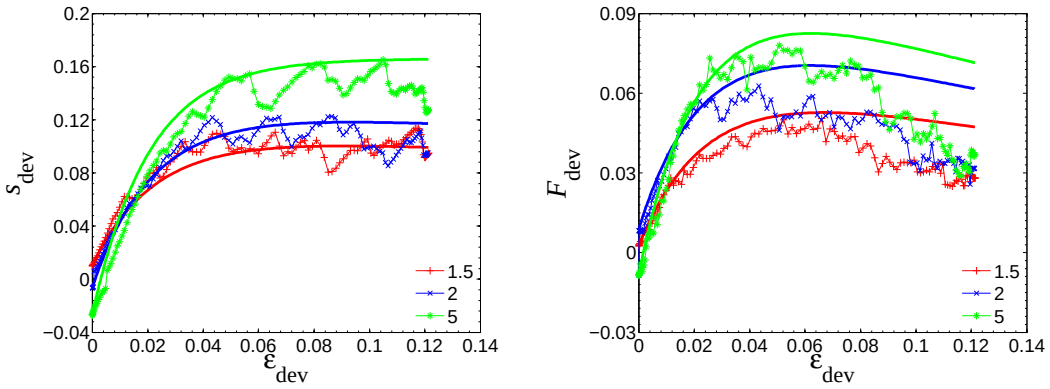
$$\mathrm{Fsgn}\left(\mathbf{Q}\right) = \mathrm{sgn}\left(Q_{yy} - Q_{xx}\right),$$

with x-wall expanding, y- compressing and a non-mobile z-wall. The sign convention explains the different initial values associated to the same initial packings in Figs. 11(a) and 12(a).



(a) (b)

Figure 11: (a) Deviatoric stress ratio $s_{\rm dev} = \sigma_{\rm dev}/P$ plotted against deviatoric strain from the deviatoric (volume conserving) mode for three polydispersities $w = 1.5$, 2 and 5 as shown in the legend. The data points are the simulation results while the solid lines through them represent fits to the data using Eq. (16). The volume fraction is $\nu = 0.75$. (b) Deviatoric fabric $F_{\rm dev}$ plotted against deviatoric strain for the same cases as in (a). The data points are simulation results while the solid lines through them are fits to the data using Eq. (17). The corresponding inset shows the behavior of growth rates β_s and β_F with isotropic fabric $F_{\rm v}$ for different w.



(a) (b)

Figure 12: (a) Deviatoric stress ratio $s_{\rm dev} = \sigma_{\rm dev}/P$ plotted against deviatoric strain from the uniaxial mode for three polydispersities $w = 1.5$, 2 and 5 as shown in the inset. The data points are the simulation results while the solid lines through them represent a prediction to the data using Eq. (16). The starting volume fraction is $\nu_i = 0.72$ and the maximum volume fraction is $\nu = 0.82$ for all the cases of polydispersity. (b) Deviatoric fabric $F_{\rm dev}$ plotted against deviatoric strain for the same cases as in (a). The data points are simulation results while the solid lines through them are the prediction using Eq. (17).

4.3.2 Effect on deviatoric Fabric

The evolution of the deviatoric fabric, $F_{\rm dev}$ as a function of the deviatoric strain $\epsilon_{\rm dev}$ is shown in Fig. 11(b) for the same deviatoric simulations as above. $F_{\rm dev}$ builds up from different random (small) initial values with rate β_F to different saturation values $F_{\rm dev}^{\rm max}$. Interestingly, the slope β_F seems to be constant (besides large fluctuations), irrespective of different polydispersity of the initial configurations. This is surprising, as the initial samples have different contact network density $F_{\rm v}$, due to polydispersity, and leads to the interesting conclusion that the incremental response of deviatoric fabric only depends on $F_{\rm dev}$ and volume fraction as state variables, while the role of the isotropic contact network is negligible. The critical value $F_{\rm dev}^{\rm max}$ shows a different trend from β_F, but similar to $s_{\rm dev}^{\rm max}$ as it increases with polydispersity

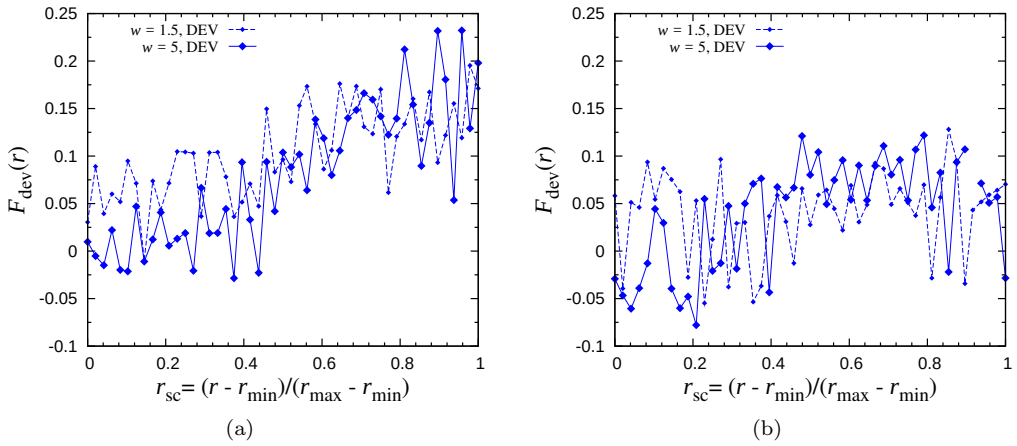


Figure 13: Deviatoric fabric per particle radius fraction $F_{\rm dev}(r)$, plotted against a scaled radius $r_{\rm sc} = (r - r_{\rm min})/(r_{\rm max} - r_{\rm min})$ for the deviatoric deformation mode, after large shear strain $\epsilon_{\rm dev} = 0.40$. Small symbols represent $w = 1.5$ and big symbols represent $w = 5$. Volume fractions are (a) $\nu = 0.686$, and (b) $\nu = 0.82$.

w. This is reasonable, when we think of the kinematics at small scale: particles with a large difference in size have more freedom to rearrange and modify the contact network during compression. The behavior of $F_{\rm dev}^{\rm max}$ is consistent with the decrease of C^* in Figs. 5(e-f), as a lower coordination number is usually associated with a higher anisotropy (La Ragione & Magnanimo, 2012).

In order to further investigate the anisotropic behavior of the material, we study the deviatoric fabric $F_{\rm dev}(r)$ per particle radius for the volume conserving deviatoric tests focusing on the large shear strain configurations, i.e. $\epsilon_{\rm dev} = 0.40$. In order to focus only on the contact orientation and not on the particle radii, we slightly modify Eq. (3) such that this quantity stays bin independent. For each radius r, we calculate

$$F_{\rm dev}(r) = (1/V)\,\frac{\sum V_r}{\sum V^{\mathcal{P}}} \sum_{\mathcal{P}\in V_r} V^{\mathcal{P}} \sum_{c\in\mathcal{P}} \mathbf{n}^c \otimes \mathbf{n}^c, \tag{14}$$

where the value of fabric is scaled by the ratio $V_r/V^{\mathcal{P}}$ between the total volume of the particles having radius r and the total volume of the particles. Please notice that Eq. (14) coincides with Eq. (3) when all the radii are considered and $\sum V_r = \sum V^{\mathcal{P}}$. In Figs. 13(a) and 13(b), we plot $F_{\rm dev}(r)$ versus the scaled radius $r_{\rm sc} = (r - r_{\rm min})/(r_{\rm max} - r_{\rm min})$ for $\nu = 0.686$ and $\nu = 0.82$. $F_{\rm dev}(r)$ increases with increasing $r_{\rm sc}$, meaning that the bigger particles form a sub-network, whose orientation follows the applied shear strain. These are the particles that belong to the force chains (Radjaï et al., 1999) and carry the majority of the applied load. On the other hand, $F_{\rm dev}(r)$ is small for small $r_{\rm sc}$, as the small particles arrange randomly, i.e. isotropically and 'caged' in the voids among the bigger particles, as already mentioned in section 4.2.2. Large fluctuations do not allow to clearly read how the behavior of $F_{\rm dev}(r)$ vs. $r_{\rm sc}$ depends on polydispersity w.

The evolution of the deviatoric fabric under uniaxial deformation is presented in Figure 12(b) for different polydispersity. In a similar fashion to deviatoric stress ratio, $F_{\rm dev}$ builds up from different (random, but small) initial values and reaches different maxima for different polydispersity, with $w = 5$ showing the highest peak, while the slope β_F stays unaffected by w. For larger strain, the structural anisotropy decreases rapidly towards zero (data not shown). This indicates that more new contacts are created in the axial direction compared to the perpendicular isotropic plane at the beginning of the loading path while at higher deviatoric strain, the fabric behaves in an opposite fashion as new contacts are created in the horizontal direction rather then in the vertical one, where most available neighbors already have come into contact. The 'softening' in deviatoric fabric does not correspond to any decrease in deviatoric stress that grows monotonically until saturation is reached (see Fig. 12(a)). The origin of this interesting feature in the uniaxial simulation, where stress and fabric show non-colinearity, and the strain eigen-system is prescribed by the wall motion, will be presented elsewhere (Imole et al., 2013).

5 Calibration of the continuum model and prediction

In this section, we will present the microscopic simulation results with a short review of an anisotropy continuum model as introduced in Luding & Perdahcıoğlu (2011). We will calibrate the free parameters in the model as function of polydispersity w and volume fraction ν, using the isotropic and purely deviatoric deformation experiments. Finally, using the model, a prediction of an independent test, i.e. the uniaxial deformation mode will be presented.

5.1 Reduced theoretical model

Most standard constitutive models with wide application fields, like elasticity, elasto-plasticity, or fluid-/gas-models of various kinds, were applied also to granular flows – sometimes with success, but typically only in a very limited range of parameters and flow conditions; for overviews see Bauer et al. (2004); Einav (2012); Göncü & Luding (2013); Imole et al. (2013); Jiang & Liu (2007); Luding & Perdahcıoğlu (2011); MiDi (2004); Tejchman & Wu (2007). While most of these theories can be and some have been extended to accommodate anisotropy of the microstructure, only very few models account for an independent evolution of the microstructure as for example Goddard (2006); Luding & Perdahcıoğlu (2011); Sun & Sundaresan (2011).

We use the constitutive model, as proposed in Luding & Perdahcıoğlu (2011), generalized for a $\mathcal{D}$-dimensional system:

$$\begin{aligned} \delta P &= \mathcal{D}B\delta\epsilon_{\rm v} + AS\delta\epsilon_{\rm dev}, \\ \delta\sigma_{\rm dev} &= A\delta\epsilon_{\rm v} + \mathcal{D}G^{\rm oct}S\delta\epsilon_{\rm dev}, \\ \delta A &= \beta_A {\rm sign}(\delta\epsilon_{\rm dev})(A^{\rm max}-A)\delta\epsilon_{\rm dev}. \end{aligned} \tag{15}$$

The model involves three moduli, namely, the classical bulk modulus B (Göncü et al., 2010), the octahedral shear modulus $G^{\rm oct}$, and the "anisotropy modulus" A. Due to the modulus A, the model provides a cross coupling between the two types of stress and strain in the model, namely the hydrostatic and the shear (deviatoric) stresses react to both isotropic and deviatoric strains. $S=(1-s_{\rm dev}/s_{\rm dev}^{\rm max})$ is an abbreviation for the stress isotropy with the stress ratio $s_{\rm dev}$ already introduced in section 4.3. The parameter $s_{\rm dev}^{\rm max}$ resembles the macroscopic friction (depending on our definition, $s_{\rm dev}=3q=3{\rm sin}\varphi$, where q is the shear stress ratio and φ is the internal friction angle as in Azéma et al. (2009) and others while β_s is the growth rate of $s_{\rm dev}$. The parameter $A^{\rm max}$ in the evolution equation of A represents the maximum anisotropy that can be reached at saturation, and $\beta_A=\beta_F$ determines how fast the asymptote is reached (growth rate) when a material is subjected to deviatoric strain $\epsilon_{\rm dev}$ (Imole et al., 2013). Both $A^{\rm max}$ and β_A are model parameters and can be extracted from fits to the macroscopic simulation results. In a nutshell, the anisotropy model is based on the basic postulate that an independent evolution of stress and structure is possible and the macroscopic modulus A accounts for the deviatoric deformation history, being proportional to the microscopic rank-two deviatoric fabric $F_{\rm dev}$. More detailed explanations about the constitutive model and its parameters can be found in Imole et al. (2013); Luding & Perdahcıoğlu (2011); Magnanimo & Luding (2011).

The reduced model, with some simplifying assumptions as introduced in Imole et al. (2013); Luding (2004, 2005b), reduces to only two independent evolution equations for the deviatoric stress ratio $s_{\rm dev}$, and the deviatoric fabric $F_{\rm dev}$, where the former is given by:

$$s_{\rm dev} = s_{\rm dev}^{\rm max} - (s_{\rm dev}^{\rm max} - s_{\rm dev}^0)e^{-\beta_s\epsilon_{\rm dev}}\,, \tag{16}$$

where $s_{\rm dev}^0$ and $s_{\rm dev}^{\rm max}$ represent the initial and maximum values of $s_{\rm dev}$ and β_s is its growth rate. Similarly, the deviatoric fabric is approximated by:

$$F_{\rm dev} = F_{\rm dev}^{\rm max} - (F_{\rm dev}^{\rm max} - F_{\rm dev}^0)e^{-\beta_F\epsilon_{\rm dev}}\,, \tag{17}$$

where $F_{\rm dev}^0$ and $F_{\rm dev}^{\rm max}$ represent the initial and maximum (saturation) values of the deviatoric fabric, and β_F is its rate of change.

5.2 Calibration for polydisperse samples

In the following, we use these two equations as empirical fit functions, since they are special cases of the complete constitutive model with anisotropy, to deduce the model parameters as functions of volume

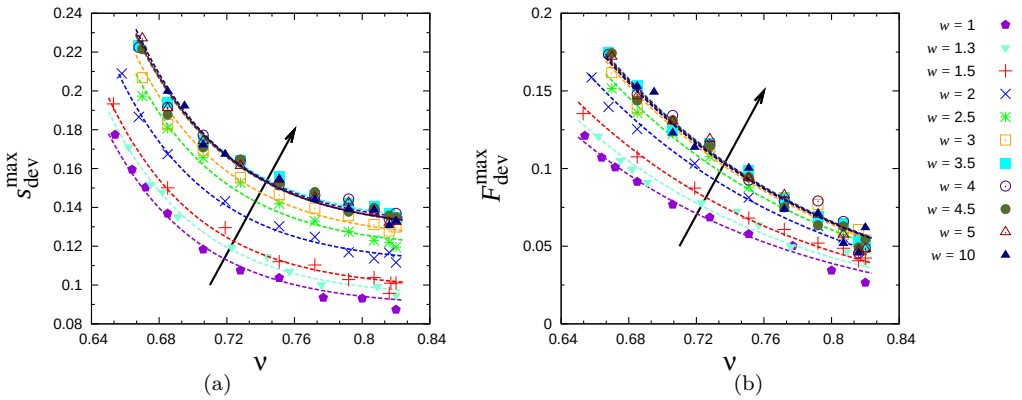


Figure 14: Comparison of evolution parameters for normalized deviatoric stress s_{dev} and F_{dev} with polydispersity w for the deviatoric deformation mode. (a) The maximum normalized deviatoric stress $s_{\mathrm{dev}}^{\mathrm{max}}$ plotted against volume fraction ν. (b) The maximum deviatoric fabric $F_{\mathrm{dev}}^{\mathrm{max}}$ plotted against volume fraction ν. The arrow indicates the increasing w. The corresponding dashed lines are the fit using Eq. (18).

fraction ν from various volume conserving deviatoric simulations (Imole et al., 2013). In particular, the influence of polydispersity w on the fitting parameters is studied. As an example, the deviatoric data for $w = 1.5$, 2 and 5 are fitted using Eqs. (16) and (17) and the four parameters $s_{\mathrm{dev}}^{\mathrm{max}}$, β_s, $F_{\mathrm{dev}}^{\mathrm{max}}$ and β_F are extracted. The procedure is applied to the full set of polydisperse packings with many different ν (not shown).

Figs. 14(a) and 14(b) show the variation of $s_{\mathrm{dev}}^{\mathrm{max}}$ and $F_{\mathrm{dev}}^{\mathrm{max}}$ respectively with ν, for different w. Both $s_{\mathrm{dev}}^{\mathrm{max}}$ and $F_{\mathrm{dev}}^{\mathrm{max}}$ decreases with increasing volume fraction ν and saturate towards a finite limit for large volume fractions. This is because for higher volume fractions, the motion of spheres is more constrained by more contacts and hence the anisotropy developed during the deformation is smaller. Moreover, with increasing polydispersity, the steady state values of $s_{\mathrm{dev}}^{\mathrm{max}}$ and $F_{\mathrm{dev}}^{\mathrm{max}}$ increase, as explained in detail in section 4.3.

Figs. 15(a) and 15(b) show the variation of β_s and β_F respectively with ν relative to the jamming volume fraction, i.e. $\nu/\nu_c - 1$, for different w from the same deviatoric simulations as above. A decreasing trend is seen for β_s versus $\nu/\nu_c - 1$, with larger scatter when compared with $s_{\mathrm{dev}}^{\mathrm{max}}$. With increasing polydispersity, the trend in the growth rate β_s with polydispersity w is minimal (this can be seen by looking at the inset in Fig. 11(a) since F_{v} in that dataset depends only on polydispersity), so we neglect this variation in this work. A similar decreasing trend in β_F with $\nu/\nu_c - 1$ is seen, while besides fluctuations, β_F is weakly dependent on w (see inset in Fig. 11(b)). In Figs. 14 and 15, we also report the values of the four parameters for the monodisperse packing, $w = 1$. We note that when β_s and β_F are plotted in Figs. 15(a) and 15(b), the data for $w = 1$ show anomalously large values. This is probably due to partial, local crystallization (Schröder-Turk et al., 2010) present in the monodisperse case.

A clear difference between the fit parameters of deviatoric stress and deviatoric fabric, namely the steady values $s_{\mathrm{dev}}^{\mathrm{max}}$, $F_{\mathrm{dev}}^{\mathrm{max}}$ (Figs. 14(a) and 14(b)), and the growth rates β_s and β_F (Figs. 15(a) and 15(b)) can be seen. This confirms that stress and fabric indeed evolve independently with deviatoric strain (Imole et al., 2013; La Ragione & Magnanimo, 2012), as is the basic postulate for the anisotropy constitutive model.

We propose a generalized analytical relation to fit the stress parameters $s_{\mathrm{dev}}^{\mathrm{max}}$, β_s and the fabric parameters $F_{\mathrm{dev}}^{\mathrm{max}}$, β_F, obtained from various different volume conserving deviatoric simulations. Their dependence on volume fraction ν (see. Imole et al. (2013), for $w = 3$), is well described by the general relation:

$$Q = Q_{\mathrm{max}}(w) + Q_{\mathrm{v}}(w) \exp\left(-\alpha(w)\left(\frac{\nu}{\nu_c(w)} - 1\right)\right) , \tag{18}$$

where $Q_{\mathrm{max}}(w)$, $Q_{\mathrm{v}}(w)$ and $\alpha(w)$ are the fitting parameters dependent on polydispersity w, with values presented in Table 3, ν is the volume fraction and $\nu_c(w)$ is the jamming volume fraction for the deviatoric deformation mode dependent on w (see Fig. 7). For all four parameters, $Q_{\mathrm{max}}(w)$ is the limit value for large volume fraction, $Q_c = Q_{\mathrm{max}}(w) + Q_{\mathrm{v}}(w)$ represents the limit at $\nu \to \nu_c(w)$, and $\alpha(w)$ is the rate

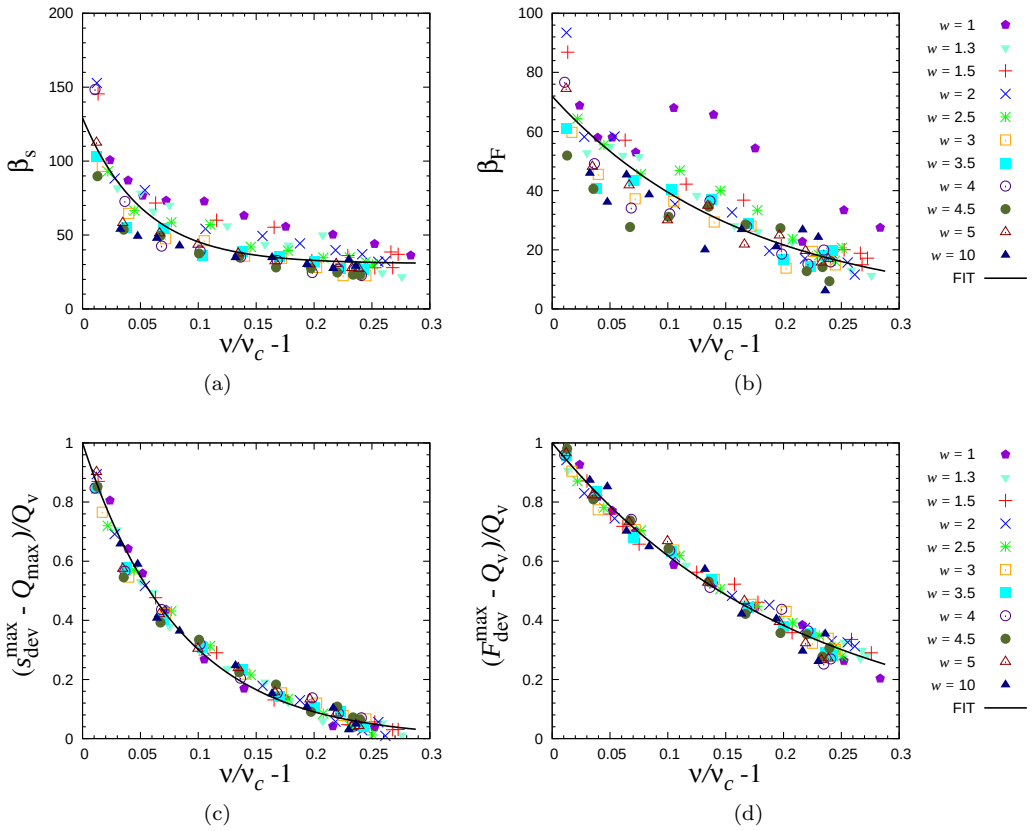


Figure 15: The growth rates (a) β_s of $s_{\rm dev}$ and (b) β_F of $F_{\rm dev}$ plotted against scaled volume fraction, $(\nu/\nu_c - 1)$. Scaled (c) $s^{\rm max}_{\rm dev}$ and (d) $F^{\rm max}_{\rm dev}$ with components $Q_{\rm max}$ and $Q_{\rm v}$ (see Table 3) plotted against scaled volume fraction, $(\nu/\nu_c - 1)$. The corresponding solid lines are the scaled parameters using Eq. (18) with data taken from Table 3.

of variation (decay) with the volume fraction.

Here we study and discuss the four cases separately. (1) For $s^{\rm max}_{\rm dev}$, from Fig. 14(a) the variation of $Q_{\rm max}$ with w is systematic and the curves are parallel. Hence $Q_{\rm v}$ and α can be considered independent of w. When the curves in $s^{\rm max}_{\rm dev}$ are scaled with the respective $Q_{\rm max}$ by $\left(s^{\rm max}_{\rm dev} - Q_{\rm max}\,(w)\right)/Q_{\rm v}$, this leads to a collapse, as shown in Fig. 15(c). (2) For β_s, in this work, we neglect its weak variation with w and assume constant values for the fit parameters $Q_{\rm max}$, $Q_{\rm v}$ and α.

When looking at the structural anisotropy, we assume, as consistent with the data, that both (3) $F^{\rm max}_{\rm dev}$ and (4) β_F tend to 0 as the volume fraction increases, therefore we set $Q_{\rm max} = 0$ in their fitting functions. We observe in Fig. 14(b), that the variation of $Q_{\rm v}$ with w is systematic for (3) $F^{\rm max}_{\rm dev}$. When $F^{\rm max}_{\rm dev}$ is scaled with $Q_{\rm v}$ by $F^{\rm max}_{\rm dev}/Q_{\rm v}\,(w)$, the data collapse as shown in Fig. 15(d). Since the curves have the same trend α is set constant independent of w. As reported in the inset of Fig. 11(b), (4) β_F is independent of the initial configuration, that is w, and we set constant $Q_{\rm v}$ and α in this case.

Interestingly, we can reduce Eq. (18) in a very compact form by expressing the two w-dependent parameters $Q_{\rm max}\,(w)$ for (1) $s^{\rm max}_{\rm dev}$, and $Q_{\rm v}\,(w)$ for (3) $F^{\rm max}_{\rm dev}$ as functions only of $\nu_c = \nu_c\,(w)$:

$$s^{\rm max}_{\rm dev}(\nu, w) = Q_{\rm max}\,(\nu_c) + Q_{\rm v}\exp(-\alpha\,(\nu/\nu_c - 1)), \tag{19a}$$

$$\beta_s(\nu, w) = Q_{\rm max} \quad + Q_{\rm v}\exp(-\alpha\,(\nu/\nu_c - 1)), \tag{19b}$$

$$F^{\rm max}_{\rm dev}(\nu, w) = \quad Q_{\rm v}\,(\nu_c)\exp(-\alpha\,(\nu/\nu_c - 1)), \tag{19c}$$

$$\beta_F(\nu, w) = \quad Q_{\rm v}\exp(-\alpha\,(\nu/\nu_c - 1)), \tag{19d}$$

with $Q_{\rm max} = -1 + 1.7\nu_c$ for (1) $s^{\rm max}_{\rm dev}$ and $Q_{\rm v} = -0.9 + 1.6\nu_c$ for (3) $F^{\rm max}_{\rm dev}$. Using these two equations, everything in Eq. (19) can be expressed as either constant, or as function of ν_c, that become a unique state variable able to describe the history of the material due to its deformation mode. Using these

		$s_{\rm dev}^{\rm max}$			$F_{\rm dev}^{\rm max}$		β_s			β_F	
w	ν_c	$Q_{\rm max}$	$Q_{\rm v}$	α	$Q_{\rm v}$	α	$Q_{\rm max}$	$Q_{\rm v}$	α	$Q_{\rm v}$	α
1.0	0.6389	0.0888			0.1308		–	–	–	–	–
1.3	0.6427	0.0935			0.1386						
1.5	0.6444	0.0976			0.1491						
2.0	0.6500	0.1106			0.1684						
2.5	0.6557	0.1164	0.11	12	0.1741	4.8	31	116	22	72	6
3.0	0.6587	0.1226			0.1789						
3.5	0.6599	0.1303			0.1830						
4.0	0.6609	0.1292			0.1810						
4.5	0.6614	0.1278			0.1777						
5.0	0.6620	0.1279			0.1782						
10.0	0.6634	0.1273			0.1751						

Table 3: Fitting coefficients for the parameters in Eqs. (16) and (17),using Eq. (18)) with $\nu_c\,(w)$, extracted from Table 4 using the deviatoric deformation mode, for various w.

equations, together with ν_c data from Table 2, and constant parameters from Table 3, we can describe the variation in the model parameters $s_{\rm dev}^{\rm max}$, β_s, $F_{\rm dev}^{\rm max}$ and β_F with volume fraction ν and polydispersity w, and use them to predict the behavior during uniaxial deformation.

5.3 Prediction of uniaxial deformation for polydisperse samples

Figure 12(a) shows the deviatoric stress ratio $s_{\rm dev}$ plotted against deviatoric strain $\epsilon_{\rm dev}$ for uniaxial deformations, compared with the predictions of Eq. (16) with coefficients $s_{\rm dev}^{\rm max}(\nu, w)$ and $\beta_s(\nu, w)$ taken from Eqs. (19a) and (19b). The proposed model, although in its simplified version, is able to properly capture the behavior of the material qualitatively, $s_{\rm dev}$ approaching exponentially a maximum value and then decreasing due to the volume fraction and polydispersity dependence of the parameters.

Figure 12(b) shows the evolution of deviatoric fabric, $F_{\rm dev}$, with deviatoric strain, $\epsilon_{\rm dev}$, for uniaxial deformations – as above – together with the predictions of Eq. (17), with parameters taken from Eqs. (19c) and (19d). The model is still able to qualitatively describe the behavior of the deviatoric fabric, but with order of 30% over-prediction for large strain. Note that the softening present in some of the deviatoric DEM data, is on purpose not plugged into the model as a constraint, which renders the weak softening present in some of the uniaxial data as a valuable prediction of the model. For better understanding, the complete coupled model needs to be used and possibly improved, as will be presented elsewhere.

6 Summary and Outlook

We use the discrete element method to investigate the behavior of three-dimensional frictionless granular assemblies characterized by different polydispersities and subjected to various deformation paths. In particular isotropic loading/unloading, deviatoric (pure) shear, and uniaxial compression are studied.

The main goal is to analyze and understand the reciprocal influence of polydispersity and deformation history on the response of the material, where the structural/bulk effects are highlighted by using the simplest linear visco-elastic contact model. The evolution of the scaled pressure as a function of volumetric strain (relative to the jamming volume fraction ν_c) is well described by an analytical (linear, to very good approximation) scaling equation (10). This shows that the isotropic fabric is proportional to the isotropic stress – when proper parameters depending slightly on the deformation mode are included. Notably, only the jamming volume fraction, among the fit parameters for the pressure, describes the role of both polydispersity and deformation history on the material behavior. As reported earlier in (Imole et al., 2013), the isotropic jamming volume fraction ν_c is not a single value for a particular

system configuration but it is strongly dependent on the deformation mode and history of the packing. Moreover, ν_c increases with polydispersity, following the behavior described in Ogarko & Luding (2012), with the isotropic and deviatoric tests giving the highest and lowest values, respectively, while the uniaxial dataset lies in between. On the contrary, the shear jamming volume fraction, slightly below the isotropic jamming volume fraction, has been confirmed as a lower limit value in recent studies, independent of the deformation path (Bi et al., 2011). The detailed simulations by Ogarko & Luding (2012), using hard instead of soft spheres, represent lower or upper bounds to ν_c if they are carried out extremely fast or slow, respectively. However, the relation between these distinct results has to be further studied elsewhere.

When the micromechanics is analyzed, the coordination number decreases with polydispersity, while the fraction of rattlers displays an opposite trend, increasing with w. In these cases, the evolution of the state variables can be predicted by using the evolution equations from (Göncü et al., 2010), with parameters dependent on the polydispersity of the packing, while the laws for the critical volume fraction $\nu_c(w)$ as extrapolated from the pressure behavior are used. Interestingly, the free fit parameters are not affected by the deformation modes in the case of the micromechanical quantities, that is they are fully described by the evolution of the critical volume fraction, acting as history variable for the sample.

The behavior of polydisperse systems are predicted by Ogarko & Luding (2012), to depend on the moments of their size distribution, after the rattlers are excluded. Since for larger w, the moments (scaled by $\langle r \rangle$) do not change much above $w \approx 3-4$, which explains the saturation of many quantitities – for the uniform size distribution used in this work.

During deviatoric and uniaxial deformations, both deviatoric stress ratio and deviatoric fabric evolve with the deviatoric strain, reaching saturation values that increase with polydispersity. The initial growth rate of stress, β_s, weakly depends on polydispersity, due to the relation between the shear stiffness of isotropic samples and the volumetric fabric $F_{\mathrm{v}}(w)$. On the other hand the growth rate of deviatoric fabric β_F is fairly independent of polydispersity (besides fluctuations), showing that the incremental response of the granular deviatoric fabric is not directly related to its isotropic state F_{v}.

The DEM data of the volume conserving deviatoric tests are used to calibrate a simple constitutive model that involves anisotropy as proposed in 2D by Luding & Perdahcıoğlu (2011); Magnanimo & Luding (2011). The four parameters that characterize the model $s_{\mathrm{dev}}^{\mathrm{max}}$, β_s $F_{\mathrm{dev}}^{\mathrm{max}}$ and β_F are expressed as functions of volume fraction and polydispersity. They show a very similar behavior decreasing with an exponential law from a maximum value at the jamming volume fraction to a saturation minimum. Also in this case, where only two parameters are depending on w and thus $\nu_c(w)$, the dependence on polydispersity can be fully described through the established variation of the jamming volume fraction $\nu_c(w)$ with w.

As final step, the constitutive model calibrated on deviatoric data is used to predict both stress and fabric evolution under uniaxial deformation – with very good qualitative success and within 70-80% quantitative agreement. The prediction of the uniaxial test shows promising perspectives for future research. The basic qualitative features are captured by the model, even though it is used in a very idealized and short form, with the single anisotropy modulus. In the future, the coupled equations have to be solved and additional formulations/terms that relate anisotropy (possibly a second anisotropy modulus) with the deviatoric fabric will also be investigated. Moreover, it would be interesting to look deeper into different distributions of polydispersity like constant volume fraction, or log-normal distributions.

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A Table of parameters

w	ν_c	p_0	γ_p	C_1	ϕ_c	ϕ_{v}
			ISO			
1.0	0.6478	0.0430	0.2131	9.0622	0.0171	46.7722
1.3	0.6491	0.0432	0.2010	9.0053	0.0220	40.5552
1.5	0.6514	0.0430	0.1698	8.9759	0.0309	35.2452
2.0	0.6577	0.0428	0.1299	8.8795	0.0650	28.6337
2.5	0.6624	0.0421	0.0499	8.7233	0.1010	20.2312
3.0	0.6648	0.0419	0.0720	8.5585	0.1559	17.6338
3.5	0.6668	0.0419	0.1481	8.4082	0.1818	13.4036
4.0	0.6674	0.0425	0.1882	8.2977	0.2049	10.5633
4.5	0.6675	0.0424	0.2409	8.1672	0.2417	9.8332
5.0	0.6680	0.0428	0.2825	8.1636	0.2513	8.0380
10.0	0.6696	0.0444	0.3992	8.1674	0.3210	4.6514
			UNI			
1.0	0.6423	0.0398	0.0776	8.7464	0.0212	39.8092
1.3	0.6440	0.0399	0.0808	8.6618	0.0254	35.2456
1.5	0.6463	0.0393	-0.0025	8.6241	0.0309	32.7265
2.0	0.6525	0.0387	-0.0840	8.5253	0.0734	26.0018
2.5	0.6576	0.0383	-0.1974	8.3847	0.1148	20.3461
3.0	0.6605	0.0376	-0.1962	8.2066	0.1640	16.0260
3.5	0.6625	0.0384	-0.0793	8.1357	0.2018	13.2581
4.0	0.6634	0.0388	0.0086	7.9881	0.2359	10.8769
4.5	0.6644	0.0390	0.0081	7.9333	0.2531	9.2102
5.0	0.6647	0.0386	-0.0527	7.8750	0.2622	7.9085
10.0	0.6662	0.0416	0.2482	7.9177	0.3342	4.4610
			DEV			
1.0	0.6389	0.0363	-0.0954	8.6689	0.0281	46.0916
1.3	0.6427	0.0405	0.1771	8.6137	0.0249	42.2059
1.5	0.6444	0.0399	0.1223	8.5451	0.0476	39.7536
2.0	0.6500	0.0387	-0.0215	8.4097	0.0744	27.1618
2.5	0.6557	0.0396	0.0594	8.3101	0.1028	19.4110
3.0	0.6587	0.0396	0.0924	8.1634	0.1453	15.2955
3.5	0.6599	0.0386	0.0382	7.9801	0.1881	12.3952
4.0	0.6609	0.0388	0.0744	7.8672	0.2131	9.8732
4.5	0.6614	0.0393	0.1539	7.7965	0.2336	8.5445
5.0	0.6620	0.0396	0.1793	7.4895	0.2492	7.3233
10.0	0.6634	0.0419	0.3617	7.7373	0.3114	3.8805

Table 4: Summary of parameters used in Eqs. (10), (12) with $C_0 = 6$, $\alpha = 0.60$ for the three modes, and (13) with polydispersity w.

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