Constitutive behavior from elementary deformation modes for assemblies of polydisperse spheres

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Abstract

The challenges of dealing with cohesive powders during storage, handling and transport are widely known in the process industries. Numerical simulations of such systems with the Discrete Element Method (DEM) provides further insight into the local micro structure of bulk materials. We present results of various deformations of dense packings of polydisperse frictionless spheres in a triaxial box and the consequences for bulk flow behaviour. We propose an objective definition for deviatoric stress and structure (anisotropy) for all deformation modes in a triaxial box and present a constitutive relation for the evolution of deviatoric stress as a function of deviatoric strain and structure according to this relation, which contains the possibility of different evolution rates.

1 Introduction and Background

The bulk behaviour of dense granular materials depends on the behaviour of their constituents (particles) interacting through contact forces. To get an understanding of the deformation behaviour of these materials, laboratory element tests can be performed. Element tests are (ideally homogeneous) macroscopic tests in which the experimentalist can control the stress or strain response path. Different element test experiments on packings of bulk solids have been realised experimentally in the biaxial box [7, 8] while other deformations modes, namely uniaxial and volume conserving shear have also been reported in [10]. While such macroscopic experiments are important in developing constitutive relations, they provide little information on the microscopic origin of the bulk flow behaviour of these complex packings. Luding et al. [5] listed four different deformation modes (0) isotropic, (1) uniaxial, (2) deviatoric (volume conserving) and (3) biaxial deformations. The former are purely strain-controlled, while the latter (3) are mixed strain-and-stress-controlled either with constant side stress [5] or constant pressure [6]. In this study, various deformation paths for aggregates of polydisperse packings of non-frictional particles are modeled using the DEM simulation approach. We study the evolution of pressure (isotropic stress) and deviatoric stress as functions of deviatoric strain, as well as structural properties like anisotropy. The final goal is to predict the macroscopic behaviour of these packings by studying their microscopic properties. We also report the evolution of deviatoric stress and deviatoric fabric as functions of deviatoric strain and will compare the evolution

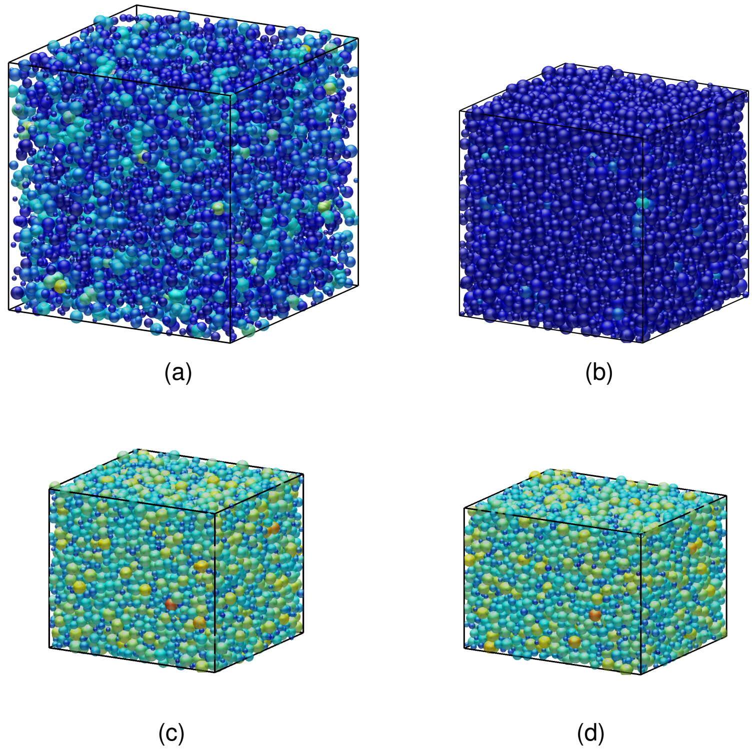

Figure 1: (a) Random positioning of particles at very low volume fraction $\phi = 0.3$; (b) particles after isotropic compression at $\phi_t < \phi_J$; (c) particles during the deviatoric (D2) loading at strain $\varepsilon_d = 0.10$; (d) particles during the same loading at strain $\varepsilon_d = 0.40$. The color code indicates particle contact strength (red: high contact, blue: no contact).

of both microstructural and stress anisotropy under deviatoric deformation with the constitutive model for volume conserving deformations proposed in [5, 6].

2 Simulation method

The Discrete Element Method (DEM) [4, 9] helps to better understand and model the constitutive behaviour of particle systems. For the sake of simplicity, the linear visco-elastic contact model for the normal component in the contact interaction between particles has been used and friction is zero (and hence no tangential component is present). The simplest normal contact force model, which takes into account excluded volume and dissipation, involves a linear repulsive and a linear dissipative force $f^n = k\delta + \gamma\dot{\delta}$, where k is the spring stiffness, γ the contact viscosity parameter and $\dot{\delta}$ is the relative velocity in the normal direction. In order to reduce dynamical effects and shorten relaxation times, an artificial viscous background dissipation force $f_b = -\gamma_b v_i$ proportional to the moving velocity v_i of particle i is added, resembling the damping due to a background medium.

Typical simulation parameters are, $N = 9261 (= 21^3)$ particles with average radius $\langle r \rangle = 1$ [mm], density $\rho = 2000$ [kg/m^3], elastic stiffness $k = 10^8$ [kg/s^2] (which determines the fastest response time scale $t_c = \pi/\sqrt{k/m} = 0.2279$ [μs] of particles with mass m), particle damping coefficient $\gamma = 1$ [kg/s], background dissipation $\gamma_b = 0.1$ [kg/s], and restitution coefficient $e =$

0.804 for two average particles. It should also be noted that the polydispersity of the system is quantified by the width $(w = r_{\max}/r_{\min} = 3)$ of a uniform distribution defined in [1, 3] where $r_{\max}$ and $r_{\min}$ are the radius of the biggest and smallest particles respectively.

3 Preparation and test procedure

For DEM simulations, the preparation step is as important as the main experiment itself. The initial configuration is such that spherical particles are randomly generated in a 3D box at a very low volume fraction $\phi = 0.3$ (ratio of the solid volume to the total volume V). This system is shown in Fig. 1(a). The system is then isotropically compressed to a target volume fraction ϕ_t below the jamming volume fraction ϕ_J, shown in Fig. 1(b). Isotropic compression is realized by a simultaneous inward movement of all the periodic boundaries of the system, with strain rate tensor $\dot{\mathbf{E}} = -\dot{\epsilon}_{\mathrm{v}}\underline{\underline{1}}$, with unit tensor $\underline{\underline{1}}$, where $\dot{\epsilon}_{\mathrm{v}}\ (>0)$ is the strain rate amplitude applied to all the walls until the target volume fraction is achieved. This is followed by a relaxation period at constant volume fraction to allow the particles to fully dissipate their energy. The system is then isotropically slowly compressed to maximum volume fraction $\phi = 0.82$ and decompression back to the volume fraction ϕ_t with small strain rate maintaining the quasi-steady of the system and this provides many possible initial configurations, both from the loading and the unloading branch.

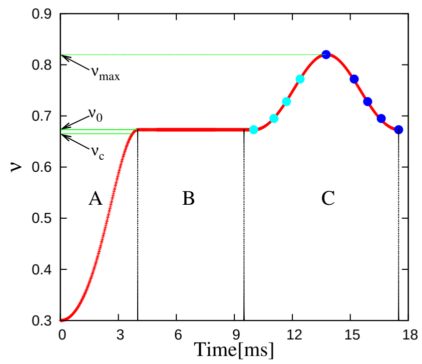

Figure 2: Evolution of volume fraction as a function of time. Region A represents the initial isotropic compression until the jamming volume fraction. B represents relaxation of the system and C represents the subsequent isotropic compression till $\nu_{\max} = 0.820$ and the decompression. The dots represent the initial configuration chosen for the deviatoric modes. Cyan dots represent the loading cycle and blue dots represent the unloading cycle.

During the previously defined isotropic 'preparation' step, we choose different initial configurations from the unloading part (represented by blue dots shown in Fig. 2) for the deviatoric simulations to test the dependence of quantities of interest on volume fraction. since it is much less sensible to the protocol and rate of deformation [1]. Then, we choose two different ways of deforming the system deviatorically. The deviatoric modes D2 and D3 have the strain rate tensors

$$\dot{\mathbf{E}} = \dot{\epsilon}_{\mathrm{D2}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \dot{\mathbf{E}} = \dot{\epsilon}_{\mathrm{D3}} \begin{pmatrix} 1/2 & 0 & 0 \\ 0 & 1/2 & 0 \\ 0 & 0 & -1 \end{pmatrix},$$

where $\dot{\epsilon}_{\mathrm{D2}}$ (> 0) and $\dot{\epsilon}_{\mathrm{D3}}$ (> 0) are the strain rate amplitudes applied for D2 and D3 modes repectively. We use the nomenclature D2/D3 since the wall motion is happening in two/three directions. In case D2, one wall moves outside as much as the other wall moves inside. In this case, D3 signifies that all the three walls are moving. In mode D3, all the three walls move with one wall twice as much as the other two (in opposite directions such that volume is conserved during deformation).

4 Results

For any deformation, the isotropic part of the infinitesimal strain tensor ϵ_{v} is defined as: $\epsilon_{\mathrm{v}} = (\epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz})/3 = \frac{1}{3}\mathrm{tr}(\mathbf{E})$, where ϵ_{xx}, ϵ_{yy} and ϵ_{zz} are the diagonal elements of the strain tensor $\mathbf{E}$ in the Cartesian-x, y and z reference system.
The average isotropic stress (pressure) is defined as: $p = (\sigma_{xx} + \sigma_{yy} + \sigma_{zz})\,3 = \mathrm{tr}(\boldsymbol{\sigma})/3$, where σ_{xx}, σ_{yy} and σ_{zz} are the diagonal elements of the stress tensor in the x, y and z reference system and $\mathrm{tr}(\boldsymbol{\sigma})$ is its trace.

Besides the stress of a static packing of powders and grains, the next most important quantity of interest is the fabric/structure tensor. For disordered media, the concept of the fabric tensor naturally occurs when the system consists of an elastic network, or a packing of discrete particles. The expression for the components of the fabric tensor is given as: $F_{\alpha\beta} = \langle F^p \rangle = \frac{1}{V}\sum_{p\in V} V^p \sum_{c=1}^{N} n_\alpha^c n_\beta^c$, where V^p is the particle volume which lies inside the averaging volume V, n_c is normal vector of particle p to contact c. $F_{\alpha\beta}$ are the components of a rank two 3x3 tensor like the stress tensor.

An objective definition of the deviatoric strain defines it in terms of the diagonal components (eigenvalues ${\epsilon_{\mathrm{d}}}^1$, ${\epsilon_{\mathrm{d}}}^2$ and ${\epsilon_{\mathrm{d}}}^3$) of the (deviatoric) tensor in its eigen system. Checking the magnitude of the off-diagonal components in the Cartesian triaxial box, one observes that those elements are negligible compared to the diagonal components, so we stick to the simpler approximate diagonal deviatoric stress definition for convenience. The results for the eigen-system orientation and analytical prediction of their magnitude will be presented elsewhere. We define the deviatoric strain magnitude as: $\varepsilon_d = \sqrt{\left((\epsilon_{xx} - \epsilon_{yy})^2 + (\epsilon_{yy} - \epsilon_{zz})^2 + (\epsilon_{zz} - \epsilon_{xx})^2\right)/2}$ where ϵ_{xx}, ϵ_{yy} and ϵ_{zz} are defined above. We define the deviatoric part of the stress (similar for deviatoric strain) as:
$\sigma_{\mathrm{dev}} = \sqrt{\left((\sigma_{xx} - \sigma_{yy})^2 + (\sigma_{yy} - \sigma_{zz})^2 + (\sigma_{zz} - \sigma_{xx})^2\right)/2}$. To quantify the anisotropy modulus in the system, we define a scalar similar to deviatoric stress and strain equation as: $F_{\mathrm{dev}} = \sqrt{\left((F_{xx} - F_{yy})^2 + (F_{yy} - F_{zz})^2 + (F_{zz} - F_{xx})^2\right)/2}$, where F_{xx}, F_{yy} and F_{zz} are the three diagonal elements of the fabric tensor.

In the following, we present the evolution of the deviatoric stress as a function of the deviatoric strain and also the evolution of the structural anisotropy. The deviatoric stress ratio ($s_{\mathrm{dev}} = \sigma_{\mathrm{dev}}/p$) quantifies the (stress) anisotropy. The loading response of the deviatoric stress for the deformation mode D2 as function of the deviatoric strain is shown in Fig. 3(a) for different volume fractions between $\nu_1 = 0.671$ to $\nu_{\max} = 0.819$ are shown. It is seen clearly that, the stresses grow initially linearly with applied strain until an asymptote (of maximum anisotropy) is reached where it remains fairly constant. The asymptote reached is a critical state of saturation and fits the constitutive model for volume conserving deformations in the biaxial box proposed in [5, 6]. Interestingly, the stress response observed from mode D3 (not shown) follows an identical path to the observations from mode D2 [3].

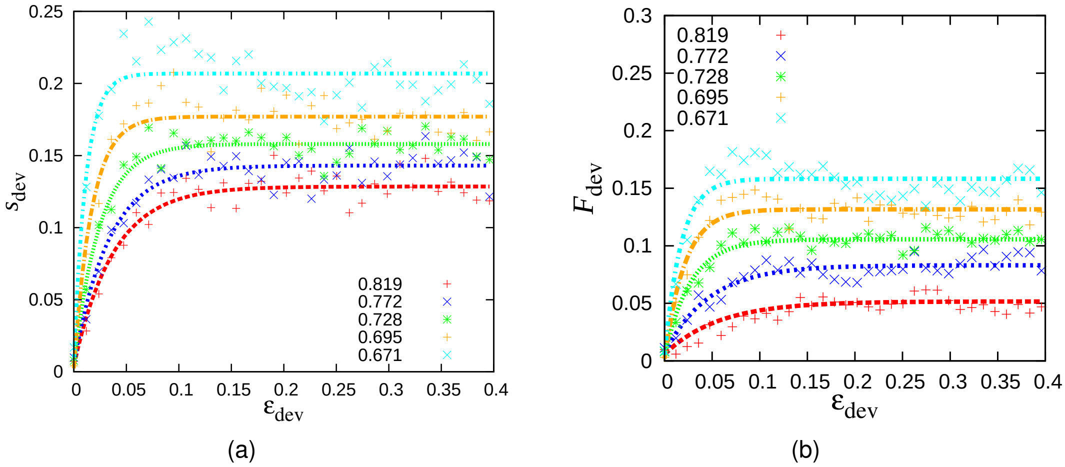

Figure 3: (a) Deviatoric stress plotted against deviatoric strain for the D2 deformation for different volume fractions. The legends gives the different initial volume fractions from which the simulations were performed. The normalized deviatoric stress increases until the saturation point is reached where additional strain does not lead to any corresponding stress response. (b) Deviatoric fabric plotted against deviatoric strain for the D2 deformation

It is noteworthy that the slope (G/p) of the normalized deviatoric stress function against deviatoric strain reduces as the volume fraction is increased, unlike the classical shear modulus G, which increases with volume fraction as consistent with findings from macroscopic experiments with shear testers. This means that the pressure increases with volume fraction faster than the shear modulus, $\mathrm{d}G/\mathrm{d}\nu < \mathrm{d}p/\mathrm{d}\nu$.
The evolution of the deviatoric fabric as a function of deviatoric strain for mode D2 is shown in Figure 3(b) for the same simulations. The deviatoric fabric builds up from different initial points to different maximum values. It also can be observed that the deviatoric fabric builds up faster for lower volume fractions. All the configurations reach then a saturation point where further deformation does not lead to an increase of the anisotropy. The evolution of the deviatoric fabric for the D3 mode is not shown since it is identical to the D2 mode implying that it is insensitive to the two deformation protocols employed.

5 Conclusion

We have presented simulation results from strain controlled deviatoric (pure shear) deformation of frictionless polydisperse spheres. For different deviatoric modes, the normalized stresses grow with strain until they reach an asymptotic value. The structural anisotropy behaves qualitatively similar but with different rates and asymptotic value. For higher volume fractions, the normalized stress values reached are smaller. Similar data can be measured from experiments with the true biaxial tester which is work-in-progress, since both deformation modes are especially simple to realise experimentally. The interplay between deviatoric strain, stress-anisotropy, and structural anisotropy is discussed in more detail in [2] and will be studied further in the future.

For further work, more realistic contact models to incorporate friction and cohesion need to be implemented. We also show results for the two different deviatoric modes.

Acknowledgement Helpful discussions with A. Singh are gratefully acknowledged. This work is supported by the European Union funded Marie Curie ITN-238577 Framework 7 (`http://www.pardem.eu/`).

References

[1] F. Göncü, O. Duran, and S. Luding. Constitutive relations for the isotropic deformation of frictionless packings of polydisperse spheres. *C. R. Mécanique*, 338(10-11):570–586, 2010.

[2] O. I. Imole, N. Kumar, V. Magnanimo, and S. Luding. Deformation modes of packings of frictionless polydisperse spheres. *KONA : Powder and Particle, submitted*, 2012.

[3] Nishant Kumar, Olukayode I. Imole, Vanessa Magnanimo, and Stefan Luding. Deformation Modes for Assemblies of Frictionless Polydisperse Spheres. *Advanced Materials Research*, 508:160–165, 2012.

[4] S. Luding. Anisotropy in cohesive, frictional granular media. *Journal of Physics: Condensed Matter*, 17(24):S2623–S2640, 2005.

[5] S. Luding and E. S. Perdahcıoğlu. A Local Constitutive Model with Anisotropy for Various Homogeneous 2D Biaxial Deformation Modes. *Chemie Ingenieur Technik*, 83(5):672–688, 2011.

[6] V. Magnanimo and S. Luding. A local constitutive model with anisotropy for ratcheting under 2D axial-symmetric isobaric deformation. *Granular Matter*, 13(3):225–232, 2011.

[7] M. Morgeneyer, L. Brendel, Z. Farkas, D. Kadau, D. E. Wolf, and J. Schwedes. Can one make a powder forget its history? *Proceedings of the 4th international conference for conveying and handling of particulate solids*, pages 12.118–12.124, 2003.

[8] M. Morgeneyer and J. Schwedes. Investigation of powder properties using alternating strain paths. *Task Quarterly*, 7(4):571–578, 2003.

[9] J. Sun and S. Sundaresan. A constitutive model with microstructure evolution for flow of rate-independent granular materials. *Journal of Fluid Mechanics*, 682:590–616, 2011.

[10] T. S. Yun and T. M. Evans. Evolution of at-rest lateral stress for cemented sands: experimental and numerical investigation. *Granular Matter*, 13(5):671–683, 2011.