

From particle simulations to macroscopic constitutive relations

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Abstract

The goal is to determine the constitutive behavior of granular packings under various deformations (isotropic and anisotropic) from particle simulations. For this we consider deformations, stress, structure and the contact forces as the basis. In a previous study [6,7] we investigated using DEM, the evolution of the coordination number (and the packing structure) and pressure as functions of the volume fraction for a polydisperse granular packing of spheres under isotropic compression. Here we focus on anisotropic deformation by implementing the triaxial test setup in a similar way. We study the effect of polydispersity changing the width of the particle size distribution. We find that an increase in polydispersity leads to a decrease in pressure at constant volume fraction whereas the macroscopic friction angle seems to increase with polydispersity. Furthermore, we performed triaxial test simulations with soft friction which is characterized by a small tangential contact stiffness. Our main observation is that using the same initial packing configuration with different friction coefficients does not lead to an obvious trend in simulation results.

Introduction

Granular matter is widely considered as a model material to understand more complex behaviour [1]. For example the concept of jamming applicable to a broad class of materials like glasses, molecular liquids or colloids is often analyzed numerically, using model systems of hard and soft spheres [2, 3]. When the size of the systems under consideration is relatively small individual particles can be tracked explicitly. However, this “microscopic” method becomes unmanageable for large scale real life applications where billions of grains are involved. Hence, macroscopic constitutive models [4] are required to relate basic mechanical properties such as stress and strain. The main drawback of the macroscopic approach is its empirical nature, which neglects microscopic particle properties and lacks physical ground, e.g., on the contact level [5].

The goal of this study is to understand the effect of polydispersity and soft interparticle friction on the macroscopic behaviour of granular materials under mechanical loading. Using the Discrete Element Method, in a previous study, isotropic deformations were studied in detail [6, 7]. Here we simulate the deformation of assemblies of particles in a triaxial test.

Simulation Setup

The assemblies consist of 9261 spherical particles initially enclosed in a cubic volume with periodic boundary conditions. The particle radius distribution function varies uniformly between r_{\min} and r_{\max} from which we define the polydispersity $w=r_{\max}/r_{\min}$. The initial packing is obtained from a dilute random granular gas (with volume fraction $v=0.3$) via isotropic compression up to $v=0.7$ and relaxation at this constant volume fraction. This configuration is then used as the starting point for further deformations. Particles interact through the simple repulsive linear spring dashpot normal contact force law and Coulomb type friction involving a (rather soft) tangential spring. In addition to the viscous damping at the contacts, (artificial) background dissipation is introduced to accelerate relaxation. For details on the contact models see [5]. Numerical values of the parameters used in the simulations are as follows: density $\rho = 2000 \text{ kg/m}^3$, average particle radius $r_{av} = 1 \text{ mm}$, spring constant $k_n = 10^8 \text{ kg/s}^2$, particle damping $\gamma_p = 1 \text{ kg/s}$, background dissipation $\gamma_b = 0.1 \text{ kg/s}$, total time of simulation $T = 5 \text{ ms}$ for one cycle of loading. These material parameters lead to the contact duration $t_c = 0.64 \mu\text{s}$ and a coefficient of restitution $e = 0.92$. The first quantity, when related to T indicates that the simulations are moderately

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slow, see Ref. [7] for a detailed study of different compression rates and their effect on the macroscopic quantities. Note that the units of time, length and mass can be scaled arbitrarily due to the simplicity of the contact model (see [5] for a discussion of the units) so that the results can be “translated” to different sizes and time-scales by re-scaling the units.

Test Setup

The triaxial test is implemented, as commonly used in the mechanics community to characterise e.g. soils. Figure 1 illustrates the test configuration at 70% filling fraction. A cosinusoidal displacement is applied on the top wall of the simulation box in the x direction, while keeping the pressure constant on the side walls. The pressure p is obtained from $(1/3)$ of the trace of the stress tensor

$$\sigma = \frac{1}{V} \sum_{c \in \mathcal{V}} l^c \otimes f^c,$$

where V is the volume occupied by the packing and l^c and f^c are the branch vector and the force at the contacts, respectively. The deviatoric stress ratio is defined as $s_D = (\sigma_1 - \sigma_2) / (\sigma_1 + \sigma_2)$ which can be related to the macroscopic friction angle, see below, where σ_1 and σ_2 are (in the triaxial configuration) practically identical to the eigenvalues of the stress tensor.

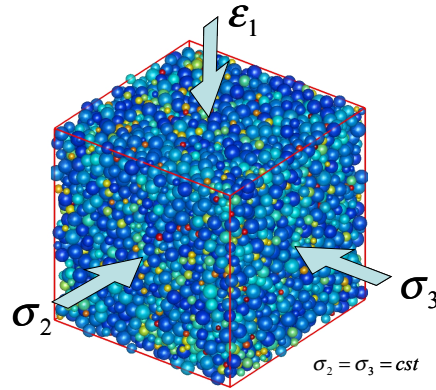


Figure 1: Initial configuration of a packing and schematic of the triaxial test implemented in the simulations. The colour code shows the pressure of individual particle. Tints of blue correspond to low and green/red indicates high pressure.

Results

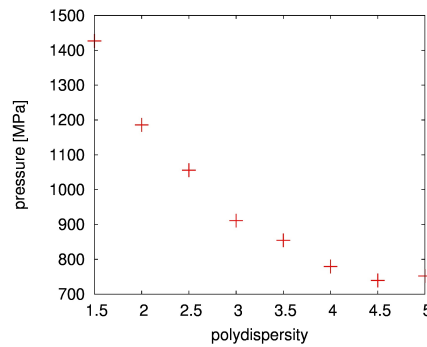


Figure 2: Relation between the initial pressure and polydispersity for packings with the same volume fraction $v = 0.7$, after isotropic compression.

Effect of polydispersity. We have performed triaxial test simulations as described above for packings with different polydispersity ranging from $w = r_{\max}/r_{\min} = 1.5$ to $w = 5$. The initial volume fraction of all packings is $v = 0.7$, however, the initial side stresses are different due to polydispersity. The three side stresses are almost identical, for one w value, but not exactly. The relation between polydispersity and

pressure is shown in Figure 2. In general, within the fluctuations, one has lower pressure for higher polydispersity, i.e. the packing is presumably more efficient.

Figure 3 (left) shows the evolution of s_D as function of the vertical strain, defined as $\varepsilon_1 = h/h_0$, where h and h_0 are the current and initial height of the box, respectively. The maximum value of s_D is related to the macroscopic friction angle defined by $\arcsin((\sigma_1 - \sigma_2)/(\sigma_1 + \sigma_2))_{\max}$. Although large fluctuations are present, the friction angle is increasing with polydispersity. The inset of Figure 3 (left) is a zoom to the small strain behaviour of s_D . Due to the above mentioned small variations in the initial stress, the initial s_D is not exactly zero. All curves start with similar slopes, i.e., polydispersity seems to have little influence on the macroscopic elastic moduli of the packing. However, note that the initial stress levels are different, so that there is no simple conclusion possible – simulations with identical stress initial conditions could help to understand this issue better.

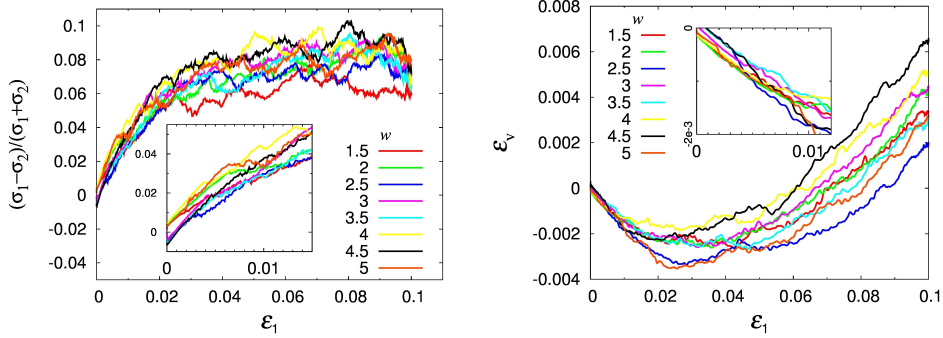


Figure 3: Triaxial test simulation results for packings, with coefficient of friction $\mu=0$ and different polydispersity w , as given in the legend. Insets: zooms to the linear regime for small ε_1 .

The volumetric strain defined by $\varepsilon_v = \varepsilon_1 + \varepsilon_2 + \varepsilon_3$ is depicted in Figure 3 (right). The small strain behavior of ε_v is shown in the inset of Figure 3 (right). Initially all curves have a similar slope indicating that the Poisson ratio is comparable for all packings (for the chosen constant volume fraction initial condition - at least). The almost constant slope during increase of ε_v implies that also the dilatancy angle is independent of the polydispersity. It is more difficult to deduce a simple relation between polydispersity and ε_v at higher strains because the effect of pressure difference (barotropy) cannot be neglected.

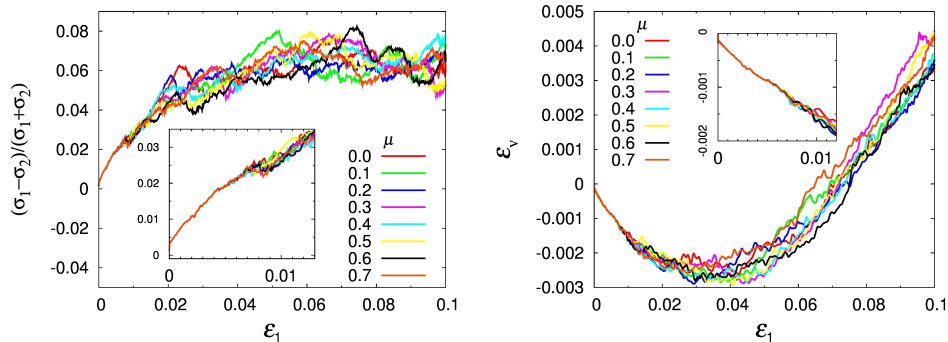


Figure 4: Triaxial test simulation results for packings with soft tangential springs $k_t/k_n = 10^{-4}$ and different interparticle friction coefficients μ , as given in the legend. Insets: zooms to the linear regime for small ε_1 .

Effect of friction. To analyze the effect of friction, we have selected an initial packing with $w=1.5$ and performed triaxial test simulations with varying coefficient of interparticle friction. Note that, friction is activated only after the triaxial test is started, hence the preparation history is the same for all packings. This has a considerable effect on the small strain behavior of the assemblies as seen in Figure 4. Again, we plot the deviatoric stress ratio s_D and the volumetric strain ε_v as functions of ε_1 . It can be seen from Figure 4 that friction has practically no effect for small strains and all curves collapse. Interparticle friction becomes important only after the first contact slip events take place in the system.

In contrast to polydispersity, it is rather difficult to observe a clear relation between the macroscopic friction angle and the interparticle coefficient of friction from the simulation results with soft tangential springs in Fig. 4 (left). Likewise, changing the friction does not lead to a clear trend in the relation between ε_v and ε_1 in Fig. 4 (right).

Summary

We have implemented the triaxial test using DEM to analyze the effect of polydispersity and “soft” friction on the macroscopic behavior of granular packings. We find that an increase in polydispersity leads to a decrease in confining pressure at constant volume fraction, after isotropic compression. Furthermore, the macroscopic friction angle increases systematically with polydispersity and the Poisson-ratio as well as the dilatancy angle seem to be independent of polydispersity. At higher strains the effect of pressure difference becomes important and it is not possible to easily relate e.g. polydispersity to the isotropic strain ε_v .

The preparation of the initial packing is also crucial for simulations with friction. Using the same initial packing at a chosen w for triaxial tests with different interparticle coefficients of friction leads to identical behaviour at small strains and non-systematic variations at larger strains. The onset of the variation sets in a little earlier with smaller coefficient of friction. Overall, we could not observe clear relations between friction and macroscopic quantities measured in simulations, when the rather small tangential spring-stiffness is used. Future work will involve “hard” friction with much larger values of the tangential stiffness.

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