

Sample preparation of dense granular materials

Influence of void ratio e and coordination number Z^* on the mechanical behaviour at failure

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Abstract. This paper presents a Discrete Element Method (DEM) study of assemblies of 5041 frictional discs, with periodic boundary conditions and confined by an external isotropic load. In order to generate samples with different internal state variables like the void ratio and coordination number, we present two different numerical procedures. The first technique, which has been widely used in the literature for many years, consists in controlling the coefficient of friction between particles to adjust the density of the samples, which directly influences the coordination number. The second technique is inspired by the previous one but adds an extra step of dynamic mixing with intergranular contacts lubrication. This makes it possible to control quasi independently the void ratio and the coordination number in the case of dense samples. These two types of samples are subjected to simple shear to analyse the influence of the sample preparation procedure on their macroscopic mechanical behaviour.

1 Introduction

In order to be able to study the mechanical behaviour of granular materials under shear, it is first necessary to prepare the samples. If they do not come from the field (by coring, for example), the samples are manufactured in the laboratory. The experimenter as well as the DEM expert then has the concern to prepare homogeneous samples for which he controls internal parameters such as density. Numerical samples have the advantage that the internal variables such as the coordination number, the contact orientations, etc. [1], are more easily accessible than for experimental samples (but possible through the use of tools such as X-rays tomography [2, 3]). Nevertheless, when the researcher wishes to explore the mechanical behaviour of granular matter, the numerical engineer has a higher number of levers at his disposal to prepare samples with a wide control of internal parameters such as void ratio e and coordination number Z^* . In addition to gravity that can be cancelled to avoid stress gradients, the DEM allows the production of extremely dense samples with perfect lubrication of the intergranular contacts (friction cancellation). The samples obtained in this way make it possible to reach densities that are very difficult to obtain experimentally. Moreover, via DEM, it is also possible to add agitation steps with perfect lubrication which allow to obtain very dense states but for which the contact networks are poorly coordinated. This technique was originally suggested by [4] on assemblies of spheres and later used by other authors like [5] for studying the influence of e and Z^* on the elastic properties of granular media. In this paper, we discuss the details of technique proposed by [4], explore its

limits and study the extent to which e and Z^* influence the mechanical strength of our granular material.

2 Model and sample preparation

2.1 The granular model

Samples of 5041 discs are generated, with grain diameters d uniformly distributed between 0.25 and 0.5. These grains interact between each other through contact points and the intergranular forces are computed when discs are in contact. Two forces are computed at the contact point: a normal elastic force, proportional to the overlap distance $\delta_N = \|\vec{r}_j - \vec{r}_i\| - R_j - R_i$ where \vec{r} and R are the position and the radius of the discs i and j , respectively. When $\delta_N < 0$, a contact occurs and the normal force is described as $f_N = -\delta k_N$. A second force is computed: the tangential force f_T that results from a sum of elastic increments $\Delta f_T = k_T \Delta_T$ over time steps (Δ_T is an increment of relative tangential displacement), the total force being limited by the Coulomb criterion, $|f_T| \leq \mu f_N$ where μ is the contact friction coefficient. The normal stiffness k_N and the tangential stiffness k_T are such that $k_T/k_N = 1$ and $\kappa = \frac{k_N}{\sigma_0} = 10000$ [6] where σ_0 is the average pressure applied on the particle assembly. The temporal discretization of the Newton equation uses a predictor-corrector scheme of order 3. The time step δt used is chosen small enough such that the discretization scheme is numerically stable. Those numerical approaches, called molecular dynamics (MD) or discrete element methods (DEM) thus rely on a dynamic approach that needs a damping energy process. Hence, a dashpot is added to the normal force law, [7]. The particle specimens are generated in an initial square virtual box where the boundaries are periodic. Hence, the

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A video is available at <https://doi.org/10.48448/6g28-7j66>

sample is in contact with itself which have the advantage of limiting the harmful effects of geometric constraints of rigid walls. Details on both the discrete element method used and the periodic boundary condition description can be found in [6].

2.2 Sample preparation

One of the objectives of the study presented here is to highlight the influence of internal state variables such as the void ratio e and coordination number Z^* on the mechanical behaviour of a granular medium subjected to a simple shear test. Also, before performing the shear tests, the samples must be prepared, i.e. they must be created and then confined under isotropic loading with $\sigma_{xx} = \sigma_{yy} = \sigma_0$.

Two types of samples (A and B) under isotropic loading are prepared. For a sample of type A, the void ratio $e = V_v/V_s$ (where V_v and V_s are the void surface and the solid phase surface respectively) and the coordination number $Z^* = 2N_C/N^*$ (where N_C is the total number of contacts between particles and N^* the total number of particles handling contact forces) are controlled by the friction coefficient between particles μ . Therefore, for a sample of type A, e and Z^* cannot be controlled independently. For $\mu = 1$, samples are loose (large e) with a small number of contacts (small Z^*). Oppositely, for $\mu = 0$, which can be seen as a perfect contacts lubrication, samples are very dense (small e) with a very large number of contacts, i.e. large Z^* (around 4). This latter type of sample is so dense that their mechanical behaviour under shear is observed to be very specific (unrealistic initial stiffness due too very high Z^* , extreme softening, etc. [1], compared to shear tests on Schneebeli rods). On the other hand, the sample preparation technique suggested by [4] makes it possible to obtain samples that are dense but for which it is possible to have a much lower Z^* . The mechanical behaviours observed for shear tests are then much closer to those observed in the laboratory on Schneebeli rods. Samples prepared with this technique are denoted B samples. The numerical procedure used to obtain A and B samples are given in detail below with successive steps.

- **S0**: 5041 Polydisperse discs are generated on a square lattice pattern. The granular sample is a gas with a large void ratio $e_0 \approx 1$.
- **S1**: The sample is shaken (under constant volume, by injecting an initial amount of kinetic energy E_c) in order to destroy the regular grid after an initial deposit until every particle has a cumulative displacement at least equal to 100 times its diameter. One should notice that this simulation is performed using the DEM approach called the *Non-Smooth Contact Dynamics* approach, [6] which has the advantage of being very efficient (on CPU time point of view) when the number of contacts tends to zero.
- **S2**: An isotropic compression with stress σ_0 is performed. Particles are here considered as frictionless particles, $\mu = 0$ such that we obtain perfect lubrication during this process. Once balanced, the sample reaches a

very dense state ($e = 0.1865$) with a maximum possible coordination number ($Z^* = 4.041$).

The main objective of B samples is to show dense samples with smallest Z^* than those obtained when isotropic compression is performed on perfectly lubricated contacts $\mu = 0$. Thus, the idea is, from step S2, to vanish every contact thanks to small dilation of the sample, to shake the sample to destroy the memory of the contact network obtained at the end of the S2 step and finally, to isotropically compress the sample by choosing an intergranular friction coefficient that will control the final Z^* .

- **S3**: A geometrical dilation is applied thanks to a homothetic transformation of the coordinates ∇ of all particles, $r' = (1 + \alpha) r$; where $\alpha > 0$ is the homothetic coefficient, chosen big enough for every contact between grains disappear after the geometrical transformation and small enough as to not increase too much e .
- **S4**: This step is identical to **S1**. The sample void ratio is denoted e_{ini} .
- **S5**: Isotropic re-compression. $\mu = \mu_{iso}$ is here chosen to control Z^* . The void ratio of the sample is denoted e_{iso} .

Following the steps **S0** to **S5**, samples B- μ_{iso} are obtained with $\mu_{iso} = 0; 0.1; 0.25; 0.5; 0.75$ and 1. For samples A- μ_{iso} , we performed steps **S0**, **S1** and **S5**. Excerpts of samples A-0 (small e_{iso} , big Z^*), B-1 (small e_{iso} , small Z^*) and A-1 (large e_{iso} , small Z^*) can be seen on the figure 1. Choosing different values of the initial void ratio e_{ini} and different values of μ_{iso} , samples A and B are obtained, table 1. One should notice that intermediate samples can also be obtained, e_{iso} being influenced by e_{ini} (through α in step **S3**) and Z^* being controlled by μ_{iso} , figure 2.

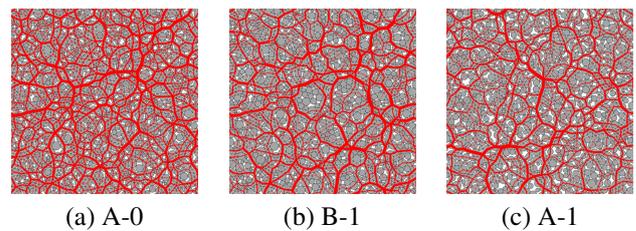


Figure 1. Excerpts of 3 samples. (a) Sample of type A-0 : $e_{iso} = 0.1865$ and $Z^* = 4.041$. (b) Sample of type B-1 : $e_{iso} = 0.1868$ and $Z^* = 3.117$, (c) Sample of type A-1 : $e_{iso} = 0.27$ and $Z^* = 3.099$

3 Simple shear tests

The simple shear tests are modelled by imposing a constant strain rate $\dot{\gamma}$ small enough to ensure a quasi-static evolution of the particles (inertial number $I = 5 \cdot 10^{-4}$, [8]). The shear tests are continued until reaching $\gamma = 0.4$ (25°). During the shear, the vertical stress is kept constant and equal to $\sigma_n = \sigma_0$ whereas the shear stress τ is computed on the full sample. During the tests, the sample surface is allowed to change. For the sake of similarity with conventional laboratory experiments on granular materials, changes in the surface of granular samples will

Table 1. Void ratio e , Contacts, rattlers (grains without contacts) proportion x_0 and coordination number Z^* for A and B samples under isotropic loading

Sample	μ_i	e	Contacts	$x_0(\%)$	Z^*
Sample A					
A-0	0	0.1865	9692	2.52	4.041
A-0.1	0.1	0.2156	8467	5.29	3.687
A-0.25	0.25	0.2413	7719	6.87	3.422
A-0.5	0.5	0.256	6885	10.56	3.192
A-0.75	0.75	0.2658	6575	12.64	3.124
A-1	1	0.27	6541	12.54	3.099
Sample B					
B-0	0	0.1842	9633	2.85	4.042
B-0.1	0.1	0.1853	8012	7.84	3.631
B-0.25	0.25	0.1859	6955	12.90	3.357
B-0.5	0.5	0.1864	6411	16.03	3.195
B-0.75	0.75	0.1867	6129	18.50	3.137
B-1	1	0.1868	6076	18.8	3.117

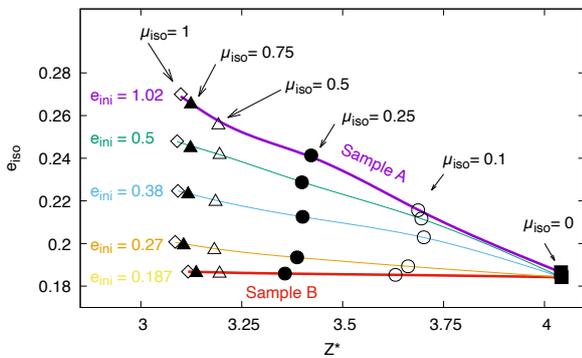


Figure 2. Relationship between the coordination number Z^* and the void ratio reach at the end of the isotropic loading e_{iso} , for samples with various initial gas void ratio e_{ini} , depending on the intergranular friction coefficient used

now be referred to as *volumetric* changes. The volumetric change is hereafter denoted as $\varepsilon_v = \Delta S/S_{iso}$, where ΔS and S_{iso} are the volume change and the volume of the sample at the start of the shear test, respectively. ε_v is a strain that is positive for compression. The evolution of the shear strength for samples of type A and B are shown on the figures 3(a) and 3(b), respectively. On the figures 3(c) and 3(d) the evolution of ε_v with respect to γ are shown. For these modelling, μ was set equal to the one used to prepare the sample, $\mu_s = \mu_{iso}$. For samples of type A, regardless of the value of μ_s , the sample strength increases until it reaches a plateau for $\gamma \geq 0.15$. We can observe that A-type samples contract until γ reaches 0.15. At $\gamma \geq 0.15$, ε_v stabilizes. These samples can be considered *loose* samples and the steady state regime observed for $\gamma > 0.15$ is the critical state. As expected, the shear tests on frictionless samples A and B show equivalent results: a limited increase in strength with almost no volumetric change ($\varepsilon_v \approx 0$), as previously explained by [9, 10].

For type B samples, the mechanical behaviour is typical of *dense* samples: they are dilatant samples until γ reaches 0.15, after which the sample volumes remain con-

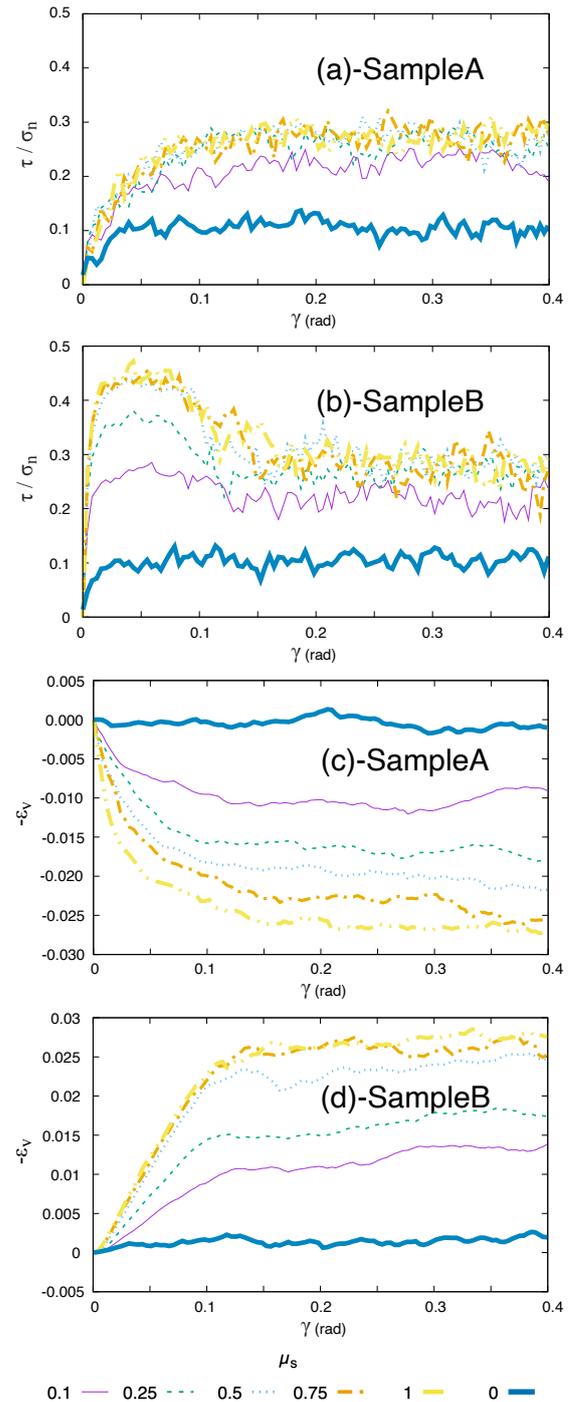


Figure 3. Relationship between stress ratio τ/σ_n and shear strain γ in figures (a) & (b) and between volumetric strain ε_v and shear strain γ in figures (c) & (d) for both samples. Value of intergranular friction during shearing is the same as the one used to prepare the sample, $\mu_{iso} = \mu_s$.

stant. For B-type samples with $\mu_s > 0$, the shear strength shows 4 phases which can be listed as hardening, peak, softening and permanent regime of constant quasi-static plastic flow. It can be noticed that whatever the value of μ_s , τ/σ_n for samples A and B are equivalent once $\gamma > 0.15$. This is consistent with the observations made by many authors: for large strains, once the permanent strength

regime reached, the internal state variables that characterize the initial state (isotropic) no longer control the mechanical behaviour – the resistance of the samples is then mainly controlled by the particle shapes and marginally by the intergranular friction coefficient [11].

4 Discussion

We discuss here the influences of the two internal state variables e_{iso} and Z^* on the mechanical behaviour of samples under shear. Many modelling were performed with various values of the intergranular friction coefficient. For example, the sample B-0, prepared using $\mu_{iso} = 0$, was used in 6 shear tests with $\mu_s = 0, 0.1, 0.25, 0.5, 0.75$ and 1. This was also done for all other B-type samples, B-0.1 to B-1, ensuring that $\mu_s \geq \mu_{iso}$, e.g., sample B-0.75 prepared with $\mu_{iso} = 0.75$ was sheared with $\mu_s = 0.75$ and $\mu_s = 1$ in two separate tests. The maximum shear strength τ_{max}/σ_0 was measured for each of these 21 shear tests and the so-called macroscopic internal angle of friction $\phi = \tan^{-1} \frac{\tau_{max}}{\sigma_0}$ was computed. These results are reported in the figure 4.

On this figure, we can observe that for a chosen μ_s , the macroscopic angle of friction corresponding to the maximum strength does not vary that much with Z^* . We can then conclude that ϕ is mainly controlled by the initial void ratio e_{iso} whereas the initial coordination number is rather controlling the amount of shear strain γ needed to reach the peak – from $(\tau/\sigma_n - \gamma)$ curves not reported in this paper.

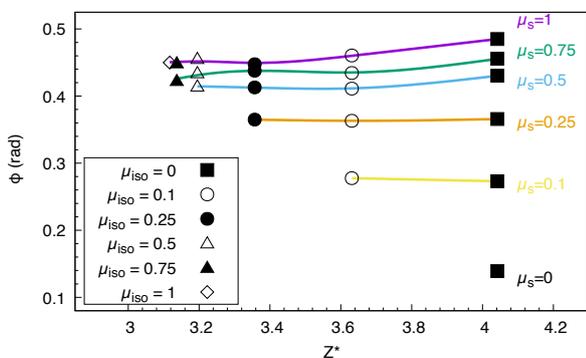


Figure 4. Macroscopic frictional angle ϕ measured at the peak strength versus Z^* for all B samples sheared with different μ_s . The colour lines indicate samples isotropically confined with various μ_{iso} but all sheared with the same friction coefficient μ_s

At this stage of the study, is it not yet possible to clearly identify which internal state parameter influences dilatancy/contractancy the most. It is clear that volumetric behaviour is dictated by the initial void ratio e_{iso} and its difference from the void ratio obtained at the end of the shear test, the void ratio at the critical state, e_c (for $\gamma > 0.15$). Knowing e_c and e_{iso} , it would be possible to easily guess if the sample will show contraction or dilation under shear. For 6 samples of type B, having almost constant void ratio e_{iso} , B-0.1 shows small dilation whereas B-1 shows strong dilation. Even if the samples are sheared with different values of the microscopic angle of friction

μ_s , the initial coordination number Z^* plays probably an important role.

5 Conclusion

The aim of the paper was to bring to light a full numerical procedure that everyone can use to generate samples confined under an isotropic loading with the advantage of a quasi-independent control of the void ratio and the coordination number. It was shown in this paper that it is possible to prepare B-type samples for which the coordination number can vary from 3 to 4 but with a constant void ratio of around 0.18, which correspond to a very dense 2D sample for the grain grading used. These granular specimens were submitted to simple shear test to study their mechanical behaviour at failure. We have shown that the maximum shear strength is essentially controlled by e_{iso} and μ_s – the initial Z^* having only a control on the macroscopic strain necessary to reach the maximum shear strength. The influence of e_{iso} and Z^* on deformation modes at grains scale (strain localization) is the next step of this study.

First author greatly acknowledges the grant from Higher Education Commission Pakistan (Grant No.5-1/HRD/UESTP/(Batch-V)/3253/2018/HEC) for their financial support during his PhD and 3SR laboratory which is part of LabEx Tec 21 (Investissements d’Avenir, grant agreement No. ANR-11-LABX-0030).

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