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DEM simulation of shear box test: discussion about the influence of initial packing.

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Abstract. The Discrete Element Method (DEM) assumes a discontinuous medium, made of particles within a granular system. Particles are represented assuming a geometric model, such as polyhedra, spheres, or another class of entities. Particles can move and interact with each other. Since the pioneer works of Cundall and Strack, the DEM has become a popular tool in scientific and industrial communities that study granular materials. Currently, despite its expensive computational cost, the utilization of DEM for the comprehension of real-world problems has gained attention. However, reproducing real problems in DEM is not a straightforward process, mainly due to several quantities of parameters such as the particle shape, materials properties, dimensions of boundaries, and number of particles. All these properties need to be defined or chosen, and they can have influence in results. Collaborating to recent discussions about good practices to model real-world problems in DEM, this paper presents the scenario of a large shear box test. A comparative analysis is done, utilizing three different particle shapes: a sphere, a convex polyhedron, and a non-convex polyhedron, addressing the effects that alterations in the initial packing of these particles have in numerical simulations results. Based on the outcomes, we can see that for the three particle shapes, the utilization of different initial packing did not present a significant impact on the variability of maximum stress and initial stiffness of the simulations. However, the modification of initial packing influenced the volumetric variation (ΔV) of samples with convex and non-convex particle shapes.

Keywords: First keyword, Second keyword, Third keyword (up to 5 keywords)

1 Introduction

Different fields, such as the pharmaceutical and food industry, railroads and highways, construction materials, and others, utilize grains as the main material in their production. Despite their pervasive use, it is known that systems composed of particles present a complex behavior, having properties similar to those observed in solids and fluids [1, 2].

Over the years, several studies have been conducted to understand the phenomena that occur in particulate systems. Some conclusions obtained by these investigations indicate that the shape [3] and size of the particles [4] are meaningful in the macroscopic behaviors of granular media.

Recently, in addition to experimental tests, the application of numerical methods to the analysis of granular materials has been considered. In this context, the Discrete Element Method (DEM), originally proposed by Cundall and Strack [5], has become a relevant tool. The DEM is formulated as a discontinuous method, where the particles present in a granular medium are represented in the simulation by numerical entities that can move freely and interact with each other, according to Newton's Laws (O'Sullivan [6]). This approach, which explicitly discretizes the particles, enables the quantification of the influence of rotations, translations, and particle contacts on the macroscopic behavior of the system analyzed (Thornton [7]).

From the user's point of view, for DEM simulations to accurately reproduce a problem, several parameters, such as particle size and shape, material properties, boundary dimensions, and the number of particles, must be accurately determined. However, the choice of these properties is not a straightforward procedure. First, because it directly influences the computational time necessary to carry out the simulations [8]. Second, obtaining some of the input parameters through experimental testing is extremely complicated, making these parameters often not measurable and their values assumed through trial and error (Coetzee [9]).

In works that employ the DEM, information about the particle shape, size distribution, and input parameters used in the numerical analysis is commonly found. The expectation is that, from this data, other users can reproduce

the same results obtained by the authors. However, it has recently been observed that in laboratory experiments and numerical simulations of triaxial tests, other parameters such as the initial particle arrangement may significantly affect the behavior of granular materials (Qian et al [10]). Looking to expand this discussion, this paper aims to investigate the effects that alterations in the initial particles' packing have on numerical simulation of large shear box tests.

2 Methodology

In our numerical analysis, three sets of simulations were carried out: the first set was composed of nine different packings, each one with 6020 convex polyhedrons identical to Figure 1a; the second set was composed of ten different packings, each one with 3651 spheres equal to Figure 1b; and the third set had eight different packings, each one with 3868 non-convex polyhedrons similar to Figure 1c.

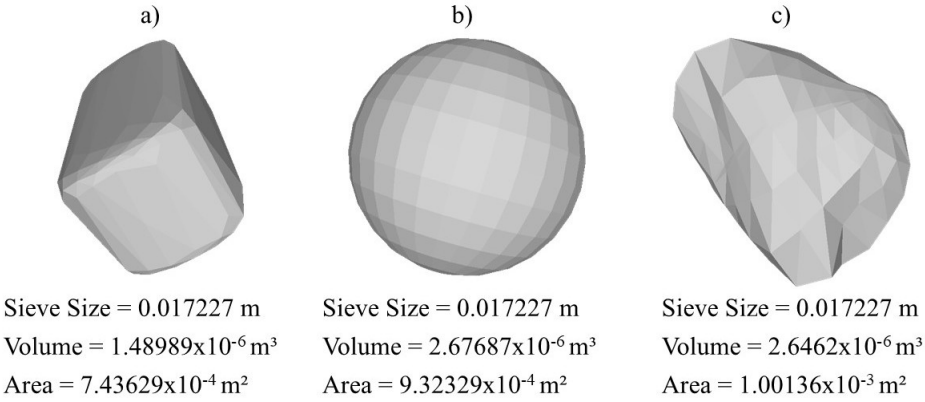


Figure 1. a) Convex polyhedron, b) sphere and c) non-convex polyhedron.

To generate each packing, the same methodology seen in Santos and Gay Neto [11] was utilized. Each packing was generated randomly, by releasing the particles in different orientations from a square hole 30 cm above the shear box base. With the particles inside the box, they were left free until all displacements and rotations disappeared. In Figure 2, the visual representations of this process are shown.

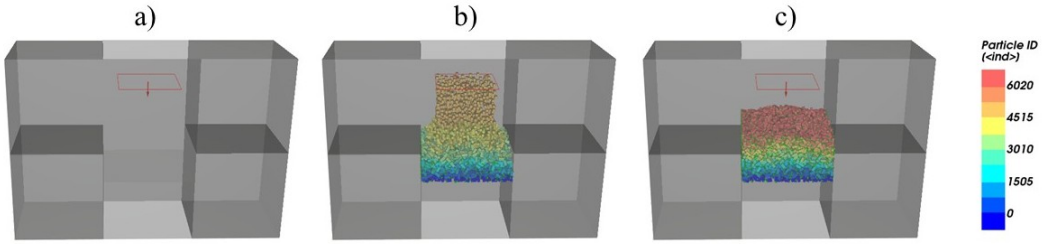


Figure 2. Random generation of particles packing: a) the shear box, b) releasing the particles, and c) example of packing utilized in simulation.

After creating the packing, a rigid plate with free vertical displacement was positioned 30 cm above the bottom of the shear box. From the positioning of the rigid plate, a downward vertical force was linearly increased during the following 2 s until a value of 9000 N was achieved in the rigid plate centroid. By applying a vertical force of 9000 N, the normal stress on the granular system equalled 100 kPa. The material was sheared by moving the bottom of the box laterally at a speed of 0.1 m/s until a total displacement of 60 mm was reached. Figure 3 shows the steps described.

To the authors' knowledge, there are no experimental results with the three types of particles shown in Figure 1. Due to the absence of experimental tests, the input material parameters, shown in Table 1, were chosen to be the same as those utilized by Santos and Gay Neto [11]. Moreover, the study used the Ansys Rocky 2024R1 and a GPU Nvidia RTX A6000 to perform the simulations.

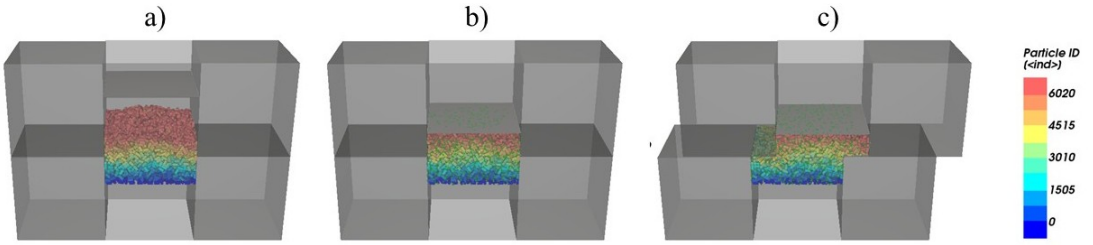


Figure 3. a) Positioning the rigid plate, b) increasing the force applied, and c) applying the lateral movement to the box.

Table 1. Input materials parameters

Model		Particle	
Gravity	9.81 m/s²	Specific mass	2700 kg/m³
Normal Contact Model	Hertzian Spring-Dashpot	Young's modulus	5 GPa
Tangential Contact Model	Linear Spring Coulomb Limit	Poisson's ratio	0.2
Rolling Contact Model (Spheres)	Linear Spring Rolling Limit	Rolling (Spheres)	0.1
Box and Plate			
Specific mass	7800 kg/m³		
Young's modulus	70 GPa		
Poisson's ratio	0.25		
Length (cm) x Width (cm)	30x30		
Particle - Particle Interactions		Particle - Boundary Interactions	
Static friction	0.90	Static friction	0.43
Dynamic friction	0.80	Dynamic friction	0.34
Tangential stiffness ratio	1	Tangential stiffness ratio	0.8
Restitution coefficient	0.1	Restitution coefficient	0.1

3 Results

To evaluate the impact of random packing generation, Table 2 shows the values of bulk density at the instant the bottom of the box began to move. These results show that, by following the steps described in Section 2, the difference in bulk density between each generated packing was less than 6%.

During the simulations, the shear stress at the shear plane and the volumetric variation (ΔV) of the particulate system were measured. The relationships found are summarized in six graphs, shown in Figure 4, where each graph groups the results of all the packings using the same type of particle.

From the curves of "Shear Stress vs Horizontal Displacement", Figures 4a, 4c, and 4e, it was possible to obtain the parameter of maximum shear stress for each packing. Analyzing by particle shape, it is possible to see that the maximum shear stress found in packings with the non-convex particle had a variation of 36.29%, with 139.909 kPa, the smallest value found, and 190.677 kPa, the largest value found. In the case of the convex polyhedron, the difference was equal to 27.05%, with 97.112 (smallest) and 123.382 kPa (largest) the values obtained by the first and fifth packing. Of the three particles analyzed, the variation of maximum shear stress between the packing of spheres showed the smallest fluctuation among the three particles analyzed. In this case, the difference found was 17.18%, with values of 139.943 kPa and 163.979 kPa for the smallest and greatest values, respectively.

Table 2. Bulk Density (kg/m³) in the simulation starts.

Packing	Convex Polyhedron	Sphere	Non-convex Polyhedron
Packing 1	1502.949	1468.619	1547.789
Packing 2	1515.061	1483.753	1552.027
Packing 3	1585.861	1480.154	1549.427
Packing 4	1527.192	1479.648	1542.857
Packing 5	1570.043	1476.767	1549.517
Packing 6	1573.700	1478.105	1552.424
Packing 7	1551.958	1478.149	1551.771
Packing 8	1556.845	1477.634	1566.614
Packing 9	1539.981	1486.406	-
Packing 10	-	1474.750	-

Besides the maximum shear strength, the residual shear stress was also analyzed. To avoid the influence of outliers, the average shear stress value was calculated for each curve within the 40–60 mm horizontal displacement interval. To the packings of the spheres and the non-convex polyhedron, the relative differences between residual shear stress were more than 40%, with 73.103 kPa the smallest and 104.049 kPa the greatest residual stress found for simulations with spheres. For the non-convex polyhedron, the smallest and greatest values were 77.392 kPa and 112.719 KPa, and the convex polyhedron had the smallest value of 74.906 kPa and the greatest 87.322 kPa.

In addition to the analysis of shear stress, Figures 4b, 4d, and 4f, show the volumetric variation of each packing during the simulation. It is possible to note that using different particle arrangements, differences in volumetric behavior of the material are obtained. Similar behavior to that expected theoretically for dense granular materials was observed for all packings of spheres and non-convex polyhedra. Interestingly, the different packing of spheres had very close results. On the other hand, the results of the convex polyhedron show that for some packings, as Packing 1, the behavior of the granular system was very different from the others, being more similar to the behavior of a material in a loose state.

4 Conclusions

By the analysis carried out, it can be seen that despite the same simulation methodology being applied, the random generation of the packings influenced the macroscopic behavior of the direct shear test results. Through this study, we have some evidence that the variability of maximum shear stress, bulk density, and residual stress found in different packings of spheres is less than that observed by other particle shapes. Furthermore, mainly in the case of the convex particle, the alteration of the packing results in a transition between the behavior expected of a granular material in a dense state to a loose state.

It should be noted that the conclusions presented are an initial analysis of the influences of packing in DEM simulations. For future works, it is recommended that the analysis be refined statistically. Another point is the possibility of verifying other combinations of parameters and packings. In addition, characteristics related to the fabric, such as the coordination, should be observed.

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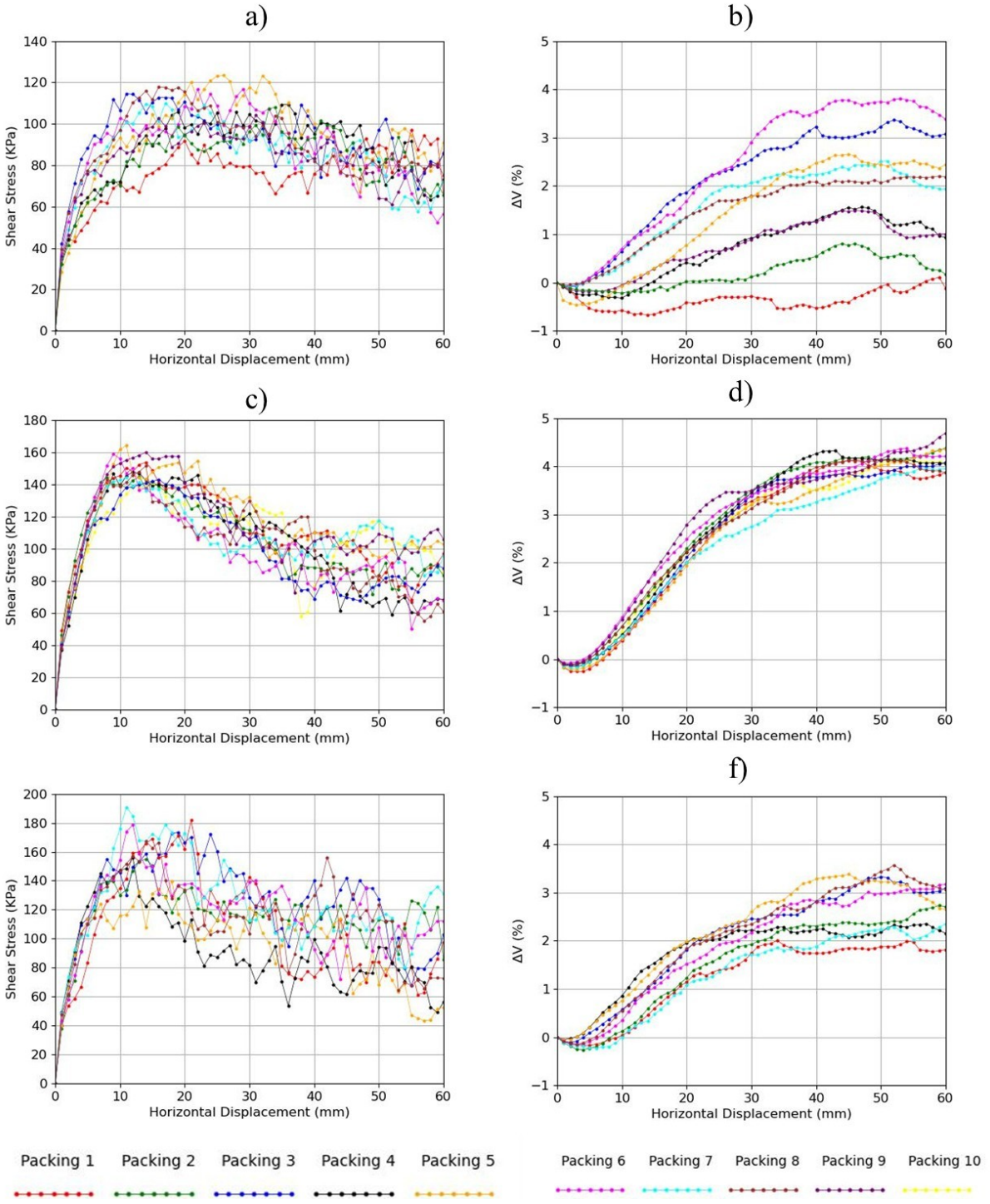


Figure 4. Simulation results: a) shear strength using the convex polyhedron, b) volumetric variation using the convex polyhedron, c) shear strength using the sphere, d) volumetric variation using the sphere, e) shear strength using the non-convex polyhedron, and f) volumetric variation using the non-convex polyhedron.

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