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A DEM study on the effect of inherent variability of assemblies of spherical particles

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ABSTRACT: This study presents DEM simulations of assemblies of spheres using periodic boundaries to assess the effect of inherent sample variability. DEM specimens with different particle size distributions (PSDs) were randomly generated, and then isotropically compressed prior to undrained (constant volume) triaxial shearing. DEM specimens with variable numbers of spheres between 500 and 10000 were generated for each PSD. Sets of simulations therefore differed only in terms of the initial, random positions of individual particles. Both macro- and micro-scale variables are then considered to assess the effect of inherent variability on the numerical results. Results indicate that all variables are significantly affected by inherent variability, however the range of variation generally decreased with an increase in specimen size. These results are some of the very first to consider the effects of sample variability that may also be intrinsically present in physical laboratory experiments on granular materials. They also highlight the importance of selecting DEM specimens of adequate size whilst considering the potential (random) variability of their mechanical behaviour.

Keywords: DEM; Variability; Specimen Generation; PSD

1 INTRODUCTION

One of the main benefits of Discrete Element Modelling (DEM), in addition to provide micro-mechanical data that is difficult to measure in an experimental manner, is its ability to reproduce repeatable results between simulations. Compared to physical experiments, in which it is essentially impossible to undertake the same test more than once and reproduce the exact same results. DEM can achieve this because once the particles and their positions have been generated, particle positions can then be re-used for multiple simulations with varying input (or simulation) parameters. From an experimental perspective, whilst it is well known that soil response is affected by sample preparation method, (e.g., Oda, 1978) it is quite difficult (and unpractical) to obtain an estimate of the variation in soil response as a result of using the same preparation procedure. In fact it is not unusual to address the repeatability of experimental results with a limited number of tests that ultimately, and at least in statistical terms, may not be representative. The shortcomming of such approach is that the effect of inherent variability has not really been addressed before in detail. Existing computational power enables researchers to systematically assess this question with different particle size distributions (PSDs) and particle counts. Furthermore, the use of periodic boundaries in DEM simulations enables this to be done free from boundary effects that may be unavoidable using experimental approaches. Finally, as a result of using this approach, questions relating to the number of particles in a simulation required to obtain a representative elementary volume (REV) in DEM simulations can also be considered.

Adesina et al., (2021) explored how many particles are required to create a statistically representative REV in 2D DEM using eliptical particles. Interestingly, a reduction in the variability between simulation results was seen as the number of particles in the REV increased. This data therefore suggests that a reduction in variability is associated with increasing particle count. Moreover, Adesina et al., (2021) stated that a reduction in the variability may be a useful metric for determining a REV. Further assessment on suitable REV size for granular materials has been performed by others (e.g. Wang et al, 2023; Omar & Sadrekarimi, 2015; Kuhn & Bagi, 2009) However, the effect of variability in DEM has never been sufficiently assessed, particularly in regard to the variation in both the macro- and micro-scale responses in 3D. The effect of PSD range has not been systematically considered either.

In this study, simulations of particle counts ranging from 500 to 10000 for two PSDs are generated and subjected to isotropic compression followed by (constant volume) undrained triaxial loading. It has been shown that denser samples exhibit fewer sample size effects in DEM as opposed to looser assemblies (e.g. Adesina et al., 2021), as such loose specimens were considered in this study. Looser specimens also benefit from faster simulation times because they (i) have less inter-particle contacts and (ii) tend to fail by instability and static liquefaction at very small strains (under undrained conditions). For the purposes of this study, analysis was undertaken by evaluating key macro and microscale parameters such as peak angle of shearing resistance (φ_{peak}), initial void ratio (e_0) and mechanical coordination numbers (Z_m).

2 DEM INPUT PARAMETERS

Simulations were performed using YADE (Šmilauer et al., 2021) and were repeated multiple times with exact specimen generation procedures. This way, differences between simulations were only in terms of initial particle positions (here referred to as inherent variability) prior to undrained shearing. DEM input parameters also remained constant throughout for the respective PSDs. In addition, the number of particles per simulation was also independently varied. The purpose of this study was therefore two-fold: (i) to estimate the number of particles required to perform a reliable and computationally efficient DEM simulation for a range of PSDs (i.e. the REV size), (ii) to quantify the extent of variability on DEM results as a consequence of inherent variability caused by random specimen generation approaches (i.e. how variable is the soil response if multiple samples/specimens are used to quantify repeatability).

A summary of DEM input parameters is shown in Table 1. These parameters where chosen to represent realistic values that have been measured experimentally by other reserachers, as discussed later. Simulations were undertaken on PSD ranges between 1 mm – 2 mm and 0.5 – 2 mm, considering a uniform distribution of particle sizes between these ranges for each sample.

Table 1. DEM input parameters

Description	**Value**
Confining stress	200 kPa
Poisson's ratio (ν)	0.22
Particle density (ρ)	2650 kg/m^3
Inter-particle friction (μ)	0.19
Young's Modulus (E)	70 GPa

The coefficient of inter-particle friction (μ) was kept constant between isotropic compression and shear, limiting this particular study to the behaviour of loose specimens, as well as preventing particle re-arrangement that would not occur in physical experiments, such as the fabric collapse due to μ reduction or sudden increase in shear stiffness upon μ increase prior to shearing.

The contact model used was the Hertzian-Mindlin contact model in the normal direction and a Coulomb-type frictional model in the shear direction, as used in many earlier DEM studies.

3 SPECIMEN GENERATION AND PROCEDURES

All specimens were radomly generated within their respective PSD range. Simulations were performed using a cubical periodic boundary of a pre-defined size (found by trial and error) that guaranteed that all particles initially fit within with no inter-particle contacts. After particle generation, a servo-controlling algorithm was used to isotropically compress specimens to the desired confining stress (200 kPa). This stage was performed for a large number of cycles that ensured the equilibrium of the specimens was reached, by using the unbalanced force ratio criterion (ratio of the maximum contact force and maximum body force). The value used here was 0.0001, much smaller than in most published DEM studies. As mentioned before, this specimen generation approach was repeated numerous times for each PSD using varying particle numbers, in order to assess the effect of the inherent variability on soil response.

Following isotropic compression, axi-symmetric compression under constant-volume (undrained) conditions was performed. The value of the maximum strain rate during shear was defined according to inertial number criteria (e.g. Da Cruz, 2005) in order to ensure quasi-static behaviour. In addition to using the faster strain rate possible, it was also decided to use loose DEM specimens (that involve a lower number of inter-particle contacts) and loading under constant volume because static liquefaction was expected at very small strain levels. This in turn enabled to perform a significantly large number of DEM simulations in an efficient manner.

4 DETERMINATION OF VARIABILITY

The variability of results was evaluated by comparing common statistical parameters such as the mean, confidence interval and coefficient of variation ($C.O.V$) for ϕ_{peak}, e_0 and Z_m, respectively, where ϕ_{peak} is the peak angle of shearing resistance, e_0 is the vois ratio after isotropic compression, and Z_m is the mechanical coordination number. Each statistical parameter is defined as follows:

$$Mean = \bar{x} = \frac{\sum x}{N} \tag{1}$$

where 'x' is the value of the parameters being assessed. Coefficient of variation ($C.O.V$):

$$C.O.V = \frac{s}{\bar{x}} \tag{2}$$

Where s is the standard deviation. The confidence interval ($C.I.$) is given by:

$$C.I = \bar{x} \pm z\frac{s}{\sqrt{n}} \quad (3)$$

where z represents the level of confidence, and n is the number of tests. The level of confidence used here was 95%.

4.1 Macroscale variability

In this section, e_0 and ϕ_{peak} are used to investigate macroscale behaviours. Figures 1 and 2 show the variability in e_0 with the number of particles (N_p) for PSDs 1 mm – 2 mm and 0.5 mm- 2 mm, respectively:

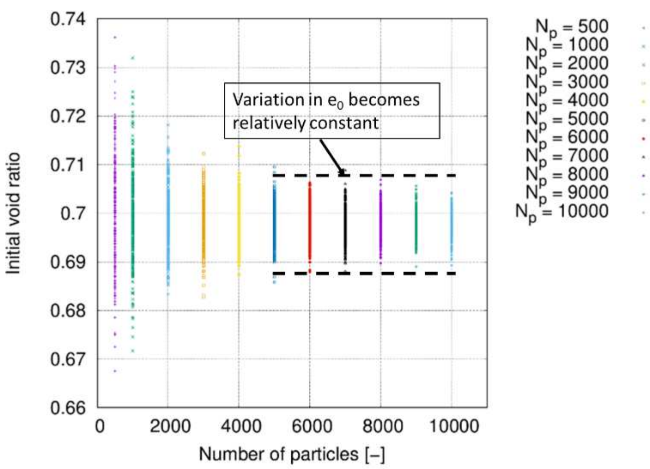

Figure 1. Initial void ratio against particle count for PSD 1 mm – 2 mm.

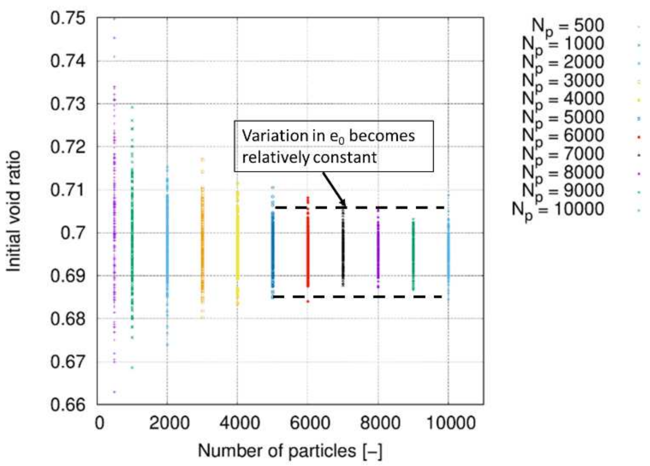

Figure 2. Initial void ratio against particle count for PSD 0.5 mm – 2 mm.

There seems to be a nigligible effect of the PSD on e_0. Note however that the variability is consistent in both PSDs, and that e_0 is slightly lower for the more poly-disperse specimens. This may result from smaller particles accommodating better between voids for the specimen within the larger diameter range.

Figures 3 and 4 show the confidence intervals for e_0 for both PSDs. In contrast to Figures 2 and 3 that illustrate individual values, Figures 3 and 4 show the variation on statistical parameters as the number of simulations were performed using the same PSD increases. The number of simulations required to achieve a $C.I$ of 0.001 (illuystared by the horizontal discontinuous black line) may be compared. For N_p = 5000 and the PSD with 1 mm – 2 mm this is approximately 120 simulations (illustrated by the vertical discontinuous black line), whilst it is much larger for the broader PSD with 0.5 mm – 2 mm (note that $C.I.$ < 0.001 is not achieved for any of the N_p values used). In other words, as the uniformity of the PSD decreases, the variability of results increases. Poly-dysperse assemblies may be considered as more "disordered" particle systems.

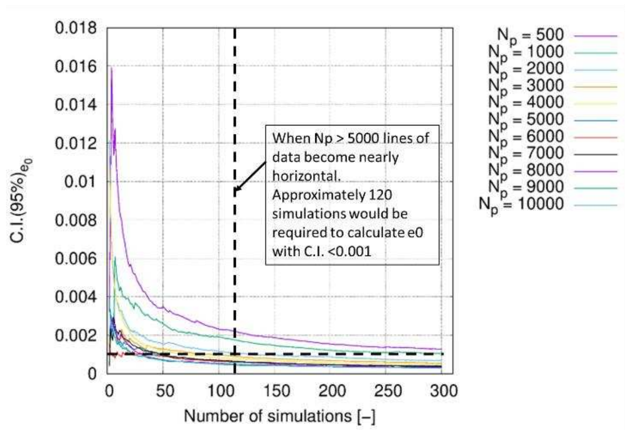

Figure 3. Confidence interval for initial void ratio for PSD 1 mm – 2 mm.

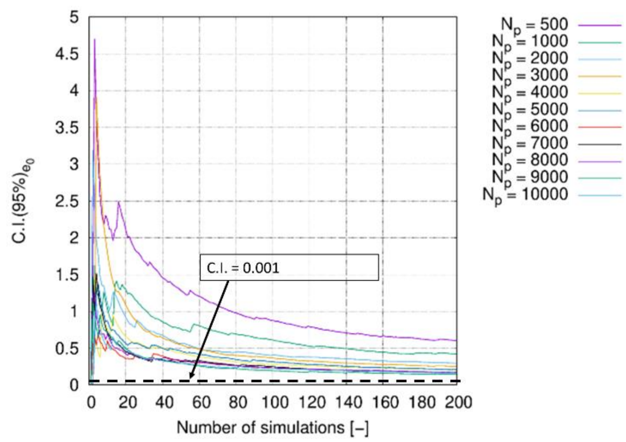

Figure 4. Confidence interval for initial void ratio for PSD 0.5 mm – 2 mm.

Figures 5 and 6 provides further clarity by plotting the $C.O.V$. In Figure 6 it can be seen clearly that for simulations with particle counts 5000 and onwards, variability reduces at around 120 simulations. Whereas in Figure 5, variation still occurs up 180-200 simulations, with significant variation occurring up until 150 simulations. The results presented here also suggest that the larger the PSD range, the larger the variability. The evolution of the mean value of ϕ_{peak} for both sets of simulations is also illustrated in Figures 7 and 8. Before analysing variability is important to note that the values of ϕ_{peak} are small compared to those that may be expected from real granular materials. The reason for this is that we have not considered particle shape effects (by simulating spheres only) and we have not included rolling resistance. Whilst is common practice by some researchers to add rolling resistance to DEM simulations on assemblies of spheres in order to get a closer quantitative agreement for ϕ_{peak}, we have avoided this because it changes soil behaviour by reducing the proportion of inter-particle sliding that would be expected in real materials (Huang et al., 2014). Furthermore, also in contrast to other earlier DEM research, we have considered more realistic and lower values for the coefficient of inter-particle friction that coincided with those that have been measured in experiments on real granualr materias (e.g. Cavarreta et al, 2010) as noted in Table 1. Nevertheless, it can be observed that the plots for 1 mm – 2 mm (Figure 7) are consistently more constant than for those of the 0.5 mm – 2 mm PSD (Figure 8). This observation is easily made by verifying the range in variation of ϕ_{peak} for each dataset, particularly as the number of simulations increases. This also further evidence that a more uniform PSD relates to lower variability.

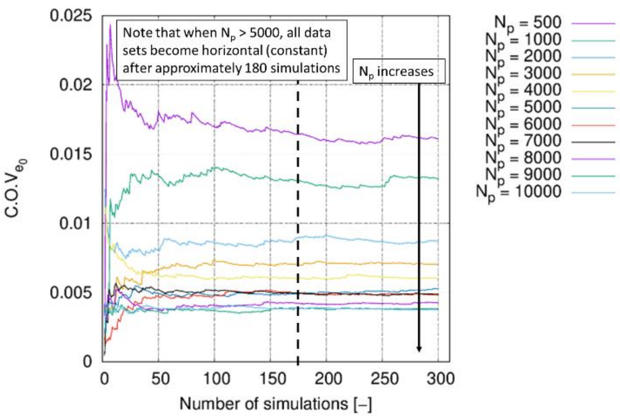

Figure 5. C.O.V for initial void ratio against number of simulations for PSD 1 mm – 2 mm.

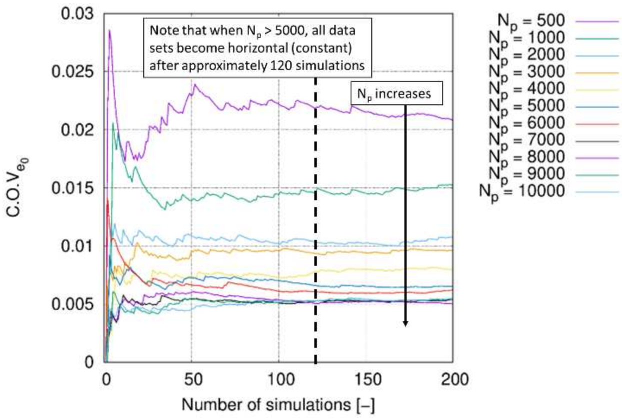

Figure 6. C.O.V for initial void ratio against number of simulations for PSD 0.5 mm – 2 mm.

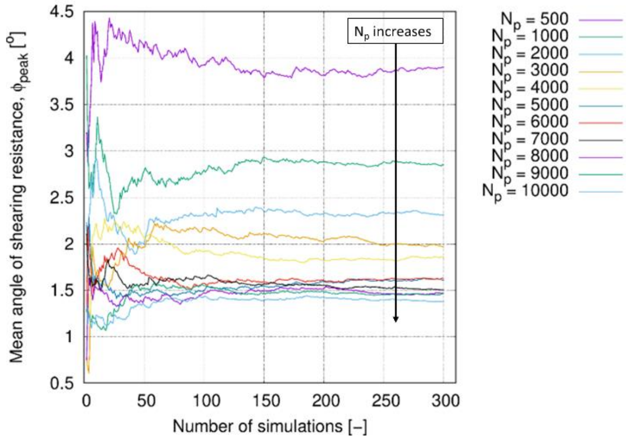

Figure 7. Mean angle of shearing resistance against number of simulations for PSD 1 mm – 2 mm.

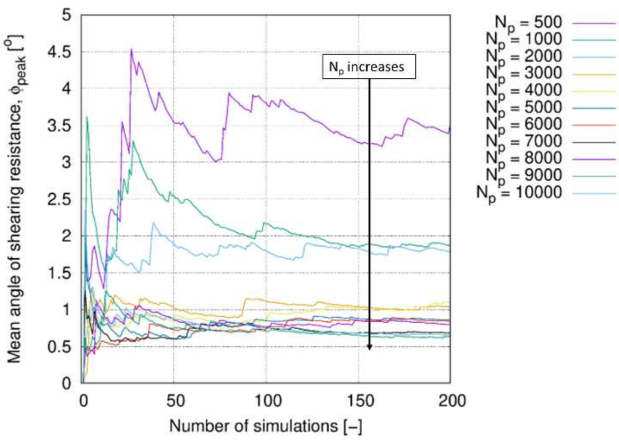

Figure 8. Mean angle of shearing resistance against number of simulations for PSD 0.5 mm – 2 mm.

4.2 Microscale variability

In regard to the microscale behaviour, Figures 9 and 10 show the mean value of Z_m after isotropic compression for both PSDs as the number of simulations considered on its calculation increases. Similar observations to those in relation to Fig.5 – 8 can be made. The range of variation for Zm in Fig. 10 is clearly higher than that observed in Figure 9. Note however, that the number of simualtions required to obatin a relatively constant value of Zm is much smaller than that observed for the macro-scale paraemeters discussed in relation to Figures 5-8. Also note that in Figure 10, the datasets for N_p = 8000 and 9000 slightly deviate the standard trend. The reason for such deviation may be of interest and it does warrant fruther investigation, however is out of scope for this study. Nevertheless, Figures 9 and 10 do indicate that (i) variability effects are present over both macro-and-micro scales; (ii) variability increases as the PSD becomes less uniform and (iii) variability reduces as the number of simualtions used to calculate a certain parameter increases.

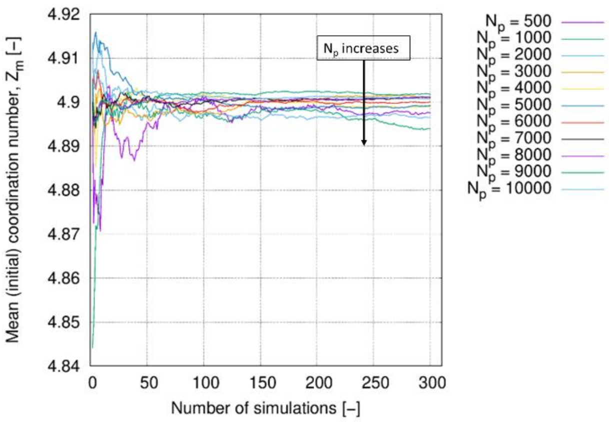

Figure 9. Mean initial coordination number against number of simulations for PSD 1 mm – 2 mm.

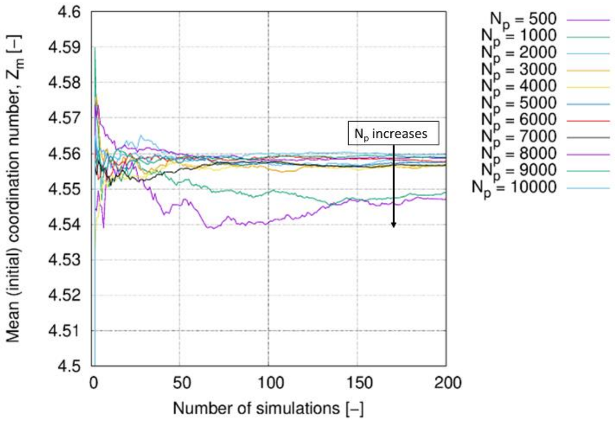

Figure 10. Mean angle of shearing resistance against number of simulations for PSD 0.5 mm – 2 mm.

In addition to Z_m, the assessment of variability in fabric, by measn of quantifying the principal values of fabric from numerically measured fabric tensor was also considered. The trends oberved were similar, in other words, showing that variability increase with PSD range, and reduces with an increase in particle numbers. However, detailed fabric analysis also enables to further analyse any kinematic constraints as the number of particles increases. These analysis are useful and interesting. They also aid to explain why variability maybe larger with smaller particle numbers, as well as larger PSD range. Such analysis is however out of scope for this paper and may be included in a different publication.

5 DISCUSSION AND CONCLUSIONS

This paper has discussed the effects of inherent variability on soil response using DEM simulations of spherical assemblies with PSD ranges of 0.5 mm – 2 mm and 1 mm – 2 mm, when sheared under undrained (constant volume) triaxial conditions. From the results presented, the following conclusions can be drawn:

- Macro-and-microscale results are both affected by inherent variability, PSD, number of particles and number of simulations performed.
- As a general trend, it is clear that the range of variation in results always reduces with an increase in both specimen size (i.e. number of particles) and number of simulations.
- The broader PSD exhibits a larger degree variability, and therefore appears to require a larger specimen size (i.e REV) than its more uniform counterparts in order to achieve statistically representative results.
- The amount of variability is also affected by the variable being quantified. For example, the variability of void ratio differs from that for coordination number and/or peak angle of shearing resistance.

Whether the results presented are applicable to other loading conditions is also an important question. Only undrained triaxial compression paths on loose three-dimensional assemblies of spheres were considered here. As discussed earlier. this was done for computational efficiency. Similar observations have been however made under drained conditions and densities by other researchers (e.g. Adesina et al., 2022). Note however that this is the first time that the PSD effect is considered. Whether the findings discussed here apply to other PSDs also warrants further investigation, together with the effects of variability of assemblies of non-spherical particles.

An important message arising from these findings goes beyond the need to accurately quantify the statistical representativeness of any DEM (or experimental) result, and the importance of choosing the right number of particles in DEM. Within an experimental context obtaining fully repeatable (with particles arranged in the same way for every sample) samples is impossible. This may also be the case in DEM (unless the same particle positions and simulations procedures are used). Consequently, it is advisable that the result of any experimental/numerical study assessing the effects of any variable (i.e. density, specimen preparation procedures, fines content, etc.) on the macro and/or microscale response of soils should always be compared against the inherent variability in order to determine how significant that effect actually is. In other words (and as an example): a DEM study that performs a parametric study on the effect particle density on soil response may obtain measurable and explainable differences as density changes. However, such differences could be smaller than those caused by inherent variability, particularly if a limited number of simulations has been performed, also with a number of particles that is not statistically representative of the given PSD. This issue may be also significant in experimental studies were testing of a significant number of repeatable samples is challenging.

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