PACIFIC EARTHQUAKE ENGINEERING RESEARCH CENTER

Micro-Inspired Continuum Modeling Using Virtual Experiments

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PEER Report No. 2022/02

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ABSTRACT

This report describes the methodology and advances reached for the project "Micro-Inspired Continuum Modeling Using Virtual Experiments." The objective of this project was to develop new hardening rules for the most common plasticity constitutive models by using accurate micromechanical simulations that can capture the main features of granular behavior under cyclic loading—a crucial feature for earthquake engineering applications. To achieve this objective, laboratory experiments were performed and scanned with X-ray computed tomography (CT). The sample processed with CT was used as input for simulations using the Level Set Discrete Element Method (LS-DEM), developed by our group. This allowed a one-to-one comparison between the individual grains of the sample and the digital twins used in the simulation. Based on our results, it was possible to observe the same dilatancy, shear banding, and cyclic changes also found in experiments. Moreover, the simulation provides the convenience of tracking the evolution of force chains and fabric tensor descriptors under loading, which is not observable from an ordinary triaxial test. The evolution of this mesoscale structure was studied to determine how it can be linked to constitutive models.

After the experiments and simulations were compared, additional analyses were done to examine fabric changes as a result of cyclic loading. Different types of samples under varied configurations were tested with LS-DEM and multiple cycles of shear and compressional loading were applied to them. As a result, evolution in coordination number, void ratio, contact fabric tensor, and force weight contact tensor were found to develop within the grains and, in some cases, cumulatively leaned to a densification of the sample over time (change in macroscopic properties from micro-scale alterations). Further testing and calibration can then be used to develop continuum formulations that relate the fabric tensor and its descriptors to cyclic constitutive models.

Keywords: continuum modeling, discrete element simulations, dilatancy, granular fabric, cyclic loading.

ACKNOWLEDGMENTS AND DISCLAIMER

This research study was partially supported by the State of California through the Transportation System Research Program of the Pacific Earthquake Engineering Research Center (PEER), under Project No. 1131- NCTRAJ. Additional support was provided by the National Science Foundation (NSF), under Grant No. 2033779. The opinions, findings, conclusions, and recommendations expressed in this publication are those of the author and do not necessarily reflect those of the funding agencies, Pacific Earthquake Engineering Research (PEER) Center, and the Regents of the University of California.

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1 INTRODUCTION

Granular fabric is a critical property to analyze when predicting the behavior of discontinuous materials such as soils, rock or ice. In essence, fabric describes the relationship among the individual objects of a granular system in terms of contacts, forces, location of voids or grain alignment. Different fabric states often lead to significant variations in granular response, such as settlement of poorly compacted soils in comparison to those with optimal packing. These effects are even more accentuated with granular materials that are of heterogenous in shape, are subjected to time-varying, or cyclic loading. Predicting performance can become challenging for these scenarios.

Micromechanically inspired continuum models have been created to predict soil mechanics behavior under complex loading such as cyclic loading. While current models such as Manzari-Dafalias (Dafalias and Manzari 2004) have the appropriate mathematical form to capture the main behavioral features in this project we propose injecting physics into the evolution laws, such as the hardening of modulus, where calibration is rather obscure due to lack of previous access to physical meaning. One aspect to specifically look at is the effect of fabric evolution and dilatancy on hardening.

The importance of fabric has been recognized and explored in experiments and models for the last two decades (Li and Dafalias 2012; Sze and Yang 2014; Vaid et al. 1999; Yamashita and Toki 1993; Yang et al. 2008). Nevertheless, further understanding of the underlying granular mechanics has been hindered, on one hand, by the lack of observation at the grain scale experimentally and, on the other hand, by the lack of accurate computational models at the grain scale (e.g., discrete element method, DEM). At the same time, natural deposition of geologic materials has been found to have significant influence in their mechanical response (Uchida et al. 2001).

In addition, experimental evidence has shown that different specimen reconstitution methods yield different mechanical responses (Dai et al. 2016; Ladd 1974; Oda 1972; Sze and Yang 2014; Tong et al. 2014; Vaid et al. 1999; Yamashita and Toki 1993), even under the "same" initial state (e.g., void ratio, stress). It stands to reason that the field and laboratory evidence is showing differences in macroscopic response that cannot be explained by our current definition of state; missing the spatial arrangement of grains and voids or fabric (Oda 1972). Unfortunately, accessing and quantifying the *in-situ* fabric is costly and fraught with difficulties due to sample disturbance (Vaid et al. 1999). It often requires the freezing of samples and requiring sophisticated experimental techniques (Oda 1972; Yang et al. 2008). The upshot of this is few and far between experiments, and our inability to study fabric effects under repeatable and controlled conditions in the laboratory, with clear implications to engineering practice (Sadrekarimi and Olson 2012), including soil seismic analysis.

As a response our group is implementing Level Set Discrete Element Method or LS-DEM to address several of the factors explained above. LS-DEM is a type of Discontinuum Computational Model that applies the principles of soft-contact DEM combined with Level Set objects to model contact interaction among granular materials rather than the usual polyhedric or spheric particle approaches. This allows LS-DEM to capture shape-related effects that can critically affect fabric descriptors. Given the use of experimentally based granular shape and fabric, virtual experiments can be developed to attain a better understanding of granular mechanics.

This project took full advantage of recent developments in accessing the grain scale from combined experimental (e.g., x-ray computed tomography, XRCT) and computational (e.g., level set discrete element method, LS-DEM) points of view. These advancements provided controlled and repeatable access to the grain scale evolution under macroscopic loading. Specifically, the proposed approach enabled us to a) develop novel methods to quantify and reconstitute the *in-situ* fabric, b) investigate the effect on fabric on the cyclic material response via virtual experiments, and c) quantify and describe fabric evolution to inform micro-inspired constitutive theories.

In order to maximize the success of the proposed research and to translate our findings to engineering practice, we performed this project in collaboration with Grenoble University (as mentioned in the proposal) and the Norwegian Geotechnical Institute (NGI) for the cyclic loading aspect through a National Science Foundation (NSF) grant. NGI, which is based in Oslo, Norway, is a geotechnical commercial foundation and international center for research and consultancy on engineering-related geosciences. NGI is interested in enhancing their understanding and improving deformation properties of granular materials for offshore applications such as offshore wind farms (OWFs).

The application of LS-DEM allows us to virtually replicate one-to-one experimental results for triaxial testing in soils. When capturing a triaxial experiment using XRCT it was possible to build a digital twin or avatar for the whole granular array that can be then simulated. In addition to obtaining and matching macroscopic indicators such as stresses and strains obtained by experiments, LS-DEM offered information on individual grains, their evolution during the experiment, as well as unobservable quantities such as rotations and intergranular contacts which are the basis for obtaining granular fabric information.

1.1 LEVEL-SET DISCRETE ELEMENT METHOD AND VIRTUAL TESTING

Investigating the behavior of granular materials purely by experiments is fraught with difficulties in creating reproducible conditions, enforcing boundary conditions, and extracting interparticle forces. An essential ingredient for constitutive modeling. The Discrete Element Method (DEM) (Cundall and Strack 1979) has provided a numerical framework that overcomes these difficulties, but at the same time, new limitations are introduced due to the idealization of granular shape. Recently, a critical advancement that can overcome these limitations has been achieved at Caltech through the level-set characterization of the exact morphology of individual grains through XRCT (Vlahinić et al. 2014), and its utilization within the Level-Set DEM (LS-DEM) framework

(Kawamoto et al. 2016). As shown in Figure 1.1., level sets are mathematical functions, whose value is the signed distance of a point to the grain's surface. Analogously to the conventional DEM, the method updates the kinematics of grains by first resolving the intergranular forces acting on discrete contact points based on the laws of contact mechanics (Kawamoto et al. 2016).

More recently, a significant step was made in validating LS-DEM under monotonic loading conditions (Kawamoto et al. 2018). The method was able to replicate an advanced high-fidelity experiment in triaxial compression equipped with sequential X-ray tomography imaging. A one-to-one virtual specimen was constructed using level-set imaging technology that allowed comparing the evolution of the volumetric strain and the stress ratio, for experiments and simulations, showing a remarkable fit. Beyond the macroscopic response, the virtual experiment was able to capture multiple aspects of the material behavior at the mesoscale. Specifically, we were able to quantitatively predict the onset and spatiotemporal evolution of the shear band and its kinematics. For example, Figure 1.2. b) compares the incremental particle rotations observed in experiment and simulation at different time stations, achieving an unprecedented prediction.

This milestone has inspired confidence, and has paved the way for a systematic investigation of granular behavior through virtual experiments, where both sample preparation and testing protocols are numerically simulated within LS-DEM. This paradigm shift frees experiments from design challenges, by allowing for boundary conditions that are hardly enforceable in a physical setting. This translates to a broad range of attainable initial material states and stress paths, that are beyond current capabilities in the laboratory. As part of this project, we aimed to push virtual experiment capabilities to general cyclic loading conditions and fully leverage this tool in an investigation of granular fabric.

1.2 CONTINUUM MODELING OF CYCLIC BEHAVIOR IN SANDS

Traditionally, the constitutive behavior of sands has been described within the context of plasticity theory. In particular, earlier models (Borja and Andrade 2006; Dafalias and Manzari 2004; Jefferies 1993) focused on achieving consistency with the Critical State Theory (CST) (Schofield and Wroth 1968), which suggests that, upon continued shear, granular materials will continue to deform at constant void ratio and pressure. Under these assumptions, the dilatancy and strength of sand depends only on the state of void ratio and pressure relevant to their critical state values (Bolton 1986), while any notion of fabric of the granular skeleton is neglected. The tendency of sands to contract or dilate, is very relevant to cyclic loading, and governs the approach to liquefaction under high magnitude excitation (Vaid and Chern 1983; Andrade et al. 2013). Not surprisingly, the predictability of earlier models was poor under general loading conditions.

More recently, there is increasing evidence from experiments and micromechanical studies that a) the monotonic cyclic response of sands is significantly affected by the initial fabric (Oda 1972; Sze and Yang 2014; Tong et al. 2014; Vaid et al. 1999; Yamashita and Toki 1993), and b) a particular fabric tends to form at critical state (Fu and Dafalias 2011; Ng 2009; Oda 1993; Oda and Iwashita 1999; Radjai et al. 2004; Wang et al. 2017; Yoshimine et al. 1998). These observations have identified the need to appropriately account for the evolution of fabric throughout the loading history of the material. To address this need, a new Anisotropic Critical State Theory (ACST) has been recently proposed (Li and Dafalias 2012), which sets the additional requirement for critical state that the soil fabric converge to a critical state value. A new family of continuum models have emerged that introduce a fabric tensor directly as a state parameter and model its evolution within ACST (Gao and Zhao 2015; Gao et al. 2014). Figure 1.3. shows the predictive capability of such a continuum model (Gao and Zhao 2015) against typical undrained cyclic triaxial experiments. It represents a clear improvement over earlier models, while still exhibiting the need for more accurate state evolution laws even within these conventional loading conditions, let alone in unconventional stress paths. The limitations of the state-of-the-art in capturing the experimental high-magnitude cyclic response are increasingly identified in recent studies (Wichtmann and Triantafyllidis 2016a, 2016b).

The response of sands sufficiently far from failure, due to lower magnitude but often high-cycle excitation, represents yet another challenge to continuum modeling. In this case, the focus of relevant continuum models lies in predicting the rate of accumulation of strain, rather than strength and dilatancy. The state-of-the-art of modeling is represented by empirical high-cycle accumulation models that introduce a creep component (Vlahinic et al. 2012; Niemunis et al. 2005). Recent studies (Wichtmann and Triantafyllidis 2017) show that the induced fabric affects significantly the accumulation of strain but is still not properly addressed by current continuum models.

CHAPTER 1: FIGURES

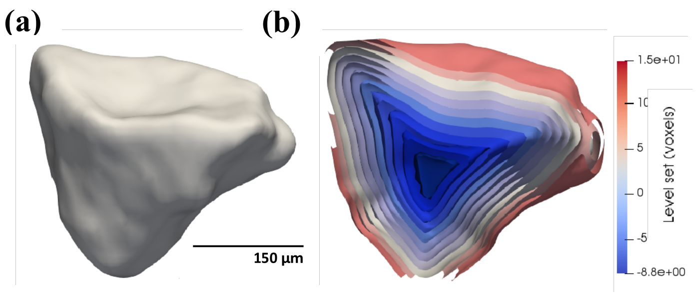

Figure 1.1 a) Hostun sand grain characterized by XRCT, and b) its level set representation.

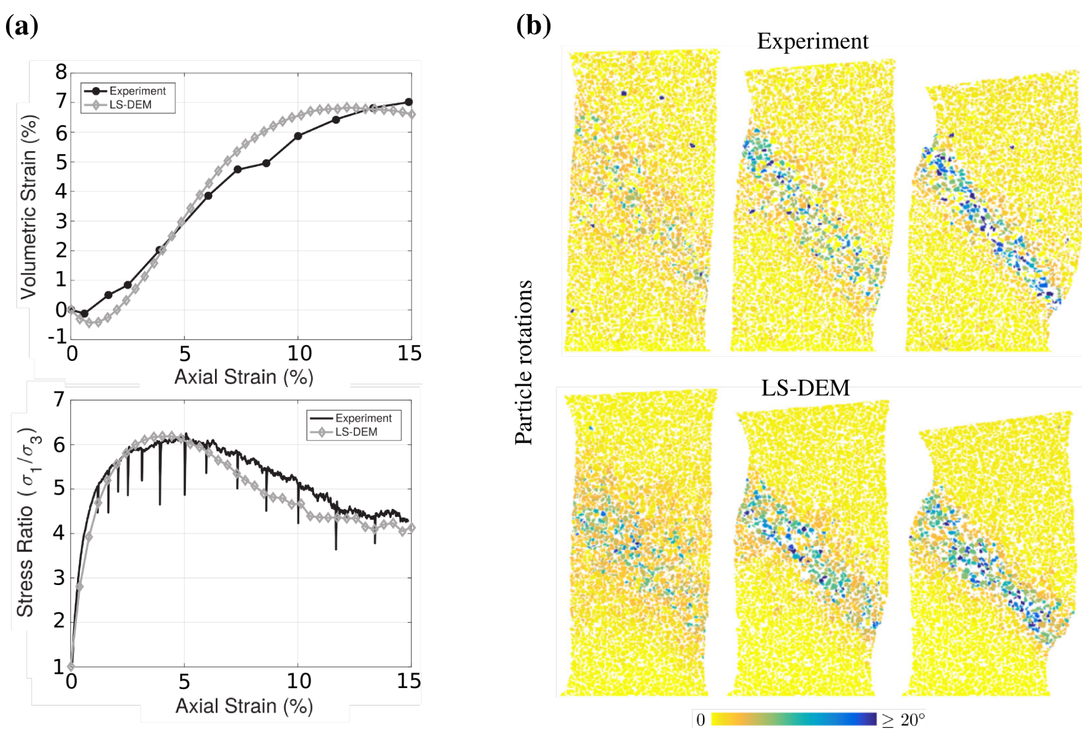

Figure 1.2 Comparison between experiment and simulation in terms of a) volumetric strain and stress ratio, both plotted against axial strain, and b) incremental particle rotations at different stages of the triaxial experiment (Kawamoto et al. 2018).

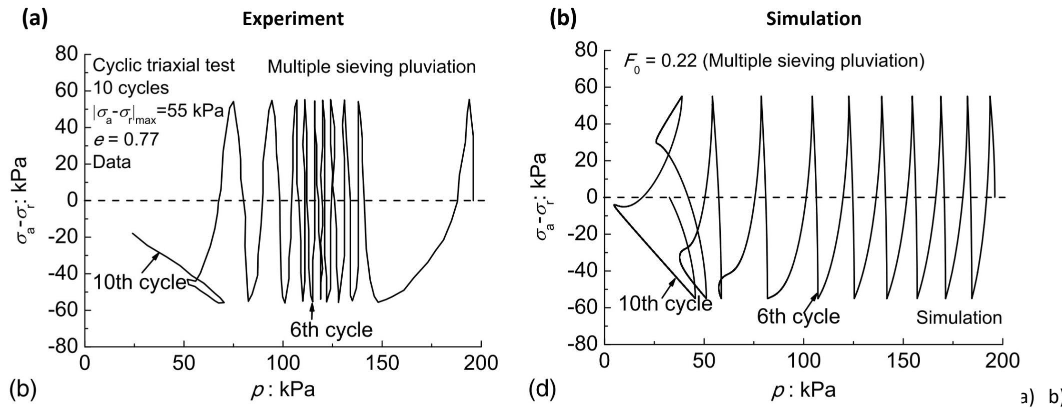

Figure 1.3 a) Experiment and b) Simulation of an undrained cyclic triaxial test using a plasticity model within the framework of anisotropic critical state theory (Gao and Zhao 2015).

2 METHODOLOGY

2.1 FROM EXPERIMENTS TO SIMULATION

Our first focus was to characterize the in-situ fabric and reconstitute it using a hybrid experimental-computational approach. Traditionally, characterization and reconstitution has targeted fabric only from the narrow perspective of void ratio. Our objective was to incorporate all aspects of the internal structure, including fabric anisotropy. The process of characterization relied on a sequence of three subtasks as shown in Figure 2.1. First, samples were physically obtained by means of ground freezing and coring techniques, in order to minimize disturbance.

The samples were thawed and scanned using high-resolution X-ray tomography. These experiments were performed with Grenoble University and involved a Caltech PhD student to translate the experimental data to simulation inputs. With the aid of imaging techniques (Vlahinić et al. 2014), the position and morphology of individual particles was extracted from XRCT data and stored (Andrade et al. 2012a, 2012b). This step involved binarizing the XRCT image via thresholding, which distinguished between voxels of solids and voids, segmenting individual grains using water shedding, and finally converting each grain into a level-set (Vlahinić et al. 2014). At this stage, by measuring the statistics of particle orientations and particle-to-particle contacts, we obtained a description of the *kinematic fabric* (i.e., the fabric described by kinematic quantities). To enhance the description of the internal structure, we generated a virtual LS-DEM specimen, where each grain was represented one-to-one in both shape and position. Once generated, the virtual sample was subjected to relaxation until any unbalanced forces, due to measurement errors, were resolved. With contact forces readily available, their statistics provided the *kinetic* or *force fabric*, completing this high-fidelity characterization procedure.

The process of reconstituting a characterized fabric relies on so-called sample reconstitution techniques, e.g., dry pluviation and moist tamping (Ladd 1974; Oda 1972; Vaid et al. 1999; Yamashita and Toki 1993). In each of the above techniques, grains are deposited in a different manner, thereby resulting in a different fabric. This is illustrated in Figure 2.2., which shows a sketch of two such techniques. We performed virtual reconstitution by utilizing LS-DEM and the grain morphologies of in-situ samples. By leveraging the resulting micromechanical output, we were able to characterize the fabric of the samples that were reconstituted with each technique, however, we decided to concentrate on dry pluviation, following the same approach as the fabric characterization of the in-situ samples. The fabric of the in-situ and the reconstituted samples were then compared, allowing us to assess the capabilities of each technique to produce the desired in-situ structure. The final evaluation of each technique will be based on the following criteria: a) ability to replicate natural depositional processes, b) sample homogeneity and test repeatability, and c) process simplicity and practicality. Upon evaluating each technique, alternative reconstitution procedures shall be proposed.

The final objective was to investigate the signature of fabric on properties that are more easily measurable in the field or the laboratory. We investigated the hypothesis that the presence of fabric induces a different response under dynamic excitation along different directions. This is tied to the concept of predicting the liquefaction potential of sands through measuring the shear wave velocity (Dobry et al. 1986; Mital et al. 2019). We took a quantitative approach, by performing virtual experiments. Samples, whose fabric has been characterized, were subjected to compressive and shear loading along different orientations in three-dimensional space.

2.2 SIMULATION CONSIDERATIONS

After translating from experiments to simulation we proceeded to carefully design physical and virtual cyclic loading experiments. First, we conducted triaxial experiments in a one-to-one fashion, where both the physical sample and its virtual counterpart (as obtained during characterization in Task 1) were subjected to the same cyclic loading program. The physical experiments were performed in-situ, i.e., inside the μXRCT apparatus. This allowed the simultaneous measurement of the macroscopic stress-strain behavior, as well as the evolution of fabric, through repeated scans during testing. The same measurements were obtained from the virtual experiments by utilizing the machinery of LS-DEM. The combination of these two techniques, provided unprecedented insight into the evolution of fabric of an in-situ specimen.

An additional outcome of this project was the enhancement of the LS-DEM code by improving its parallelization for use on high-performance computers. Currently, a single LS-DEM simulation of a triaxial test takes 17 hours to complete using 480 cores (Kawamoto et al. 2018). Even though this is longer than a single triaxial test, the numerical simulation requires no physical preparation nor clean-up. Most high-performance computing facilities will allow multiple simulations using several hundred cores to run simultaneously. In other words, several LS-DEM simulations of a triaxial test may be run simultaneously within 17 hours without the user needing to actively tend to the simulations. Physical triaxial tests, on the other hand, are limited by physical laboratory space and require active handling to clean up and prepare new tests. When combining a standard triaxial test with incremental μXRCT scans, the triaxial test may take 2-3 days. LS-DEM with its current parallelization is faster than performing physical experiments in a μXRCT apparatus while also providing valuable quantitative information about the intergranular contact forces. Therefore, the computational costs of LS-DEM in this project, especially considering the added data that it provides over physical experiments, are considered reasonable with its current parallelization, and additional enhancement of its parallelization will enhance its value in this line of research.

In a second set of virtual experiments, we applied the techniques developed to construct a set of specimens with different experimental configurations, but with similar characteristics (grain morphology, grain size distribution, void ratio). This allowed us to isolate the effect of the initial fabric in the material response and its evolution under cyclic loading conditions. Suitable mixed boundary conditions (displacement, pressure) ensured that general stress paths could be achieved. This allowed us to impose conditions found in conventional experiments, but also conditions that were traditionally unattainable in the laboratory. An example of a virtual cyclic triaxial experiment is given in Figure 2.3., which shows an isotropically consolidated sample of Hostun sand subjected to cyclic loading. Figure 2.4 compares cyclic simulations using LS-DEM against experiments carried out in NGI, showing a very good match. We have highlighted the phase transformation which is a signature of a changing fabric during the so-called cyclic mobility. Beyond conventional triaxial experiments, we conducted true triaxial experiments to investigate more general loading conditions including a) variable intermediate principal stress, and b) rotation of principal stresses under high-magnitude loading. The latter is postulated to be representative of field conditions in the case of OWFs but is difficult to attain through physical experiments.

A final set of experiments focused further on low-magnitude high-cycle loading, which has been poorly investigated in the literature, but is representative of service loading conditions in offshore structures. We focused on identifying the conditions, under which a transition occurs between continuous accumulation of deformation (ratcheting) (Alonso-Marroquín and Herrmann 2004; McNamara et al. 2008) and cyclic steady state (shakedown) (David et al. 2005; García-Rojo and Herrmann 2005; Katzenbach and Festag 2004). We will investigate the hypothesis that rate of strain accumulation is affected by the induced anisotropy, which describes the memory of the material. The output of the above experiments involves, beyond the conventional macroscopic quantities of stress and strain, the full micromechanical information including the kinematics of individual grains and the changing contact structure and contact forces. Throughout each experiment, these micromechanical quantities were continuously monitored and stored, and their statistics will provide a continuum description of fabric. Note that, contact forces are not available in conventional experimental methods (based on XRCT), thus leading to a limited description of fabric. In contrast, the proposed approach provides unprecedented access to the force fabric. Transitioning from low-magnitude high-cycle loading to high-magnitude low-frequency loading is also included in this set of additional experiments.

2.3 CONTINUUM DESCRIPTION AND FABRIC EVOLUTION

To describe material response from a continuum perspective using micro-mechanics, it is necessary to a) discover a fabric evolution law from the data, and b) rigorously validate this law. The latter is intended as a theoretical enhancement of current constitutive theories that incorporates explicitly the granular fabric and its evolution.

A comprehensive description of fabric anisotropy requires the consideration of the statistics of directional entities or fabric descriptors. Despite significant amount of research since the introduction of the concept of fabric (Oda et al. 1982; Satake 1982), the question of which descriptor is the most relevant to the continuum response remains open in the literature. As shown in Figure 2.5., we investigated several candidate descriptors including contact forces ($\mathbf{f}^c$), contact normals ($\mathbf{n}^c$), particle long-axis orientation ($\mathbf{n}^p$) (Oda 1972), as well as void vectors ($\mathbf{n}^v$) arising from an appropriate tessellation of the assembly (Li and Li 2009; Satake 1993). Given the conditions of the virtual experiments we concentrated on analyzing the former two.

The rate of evolution of the fabric potentially depends on the state and history of the material, as well as the imposed instantaneous loading. For example, preliminary observations have shown that the fabric tends to reorient itself in the direction of major principal stress, and eventually saturate upon continued shearing. At the same time, the rate at which the fabric evolves, potentially depends on the structure and the state of stress. Recently there have been significant efforts along this direction (Gao et al. 2014; Li and Dafalias 2012), however, they are predominantly inspired by monotonic responses that often rely only on the kinematic fabric and are limited by assumptions of fixed principal stress conditions. Instead, by considering the complete description of fabric, and systematically probing this relation under general cyclic loading conditions we can focus on discovering an evolution law that is general, and free of unphysical parameters. Machine learning techniques could also prove beneficial in identifying the dependence of the fabric evolution law on various stated variables.

CHAPTER 2: FIGURES

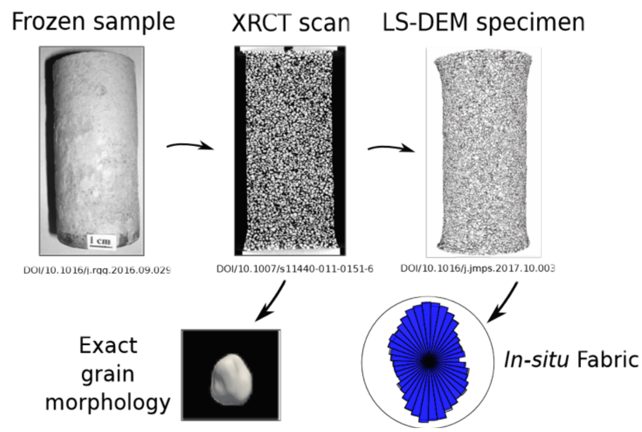

Figure 2.1 The three-step process for high-fidelity characterization of inherent fabric.

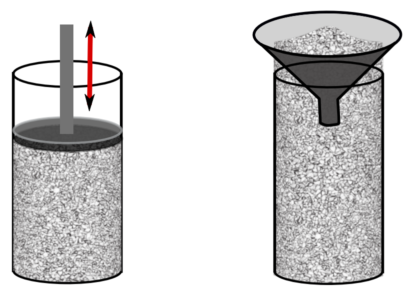

Figure 2.2 Sample reconstitution using moist tamping and dry pluviation.

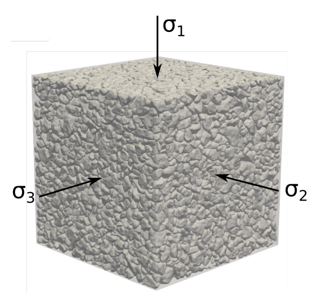

Figure 2.3 Virtual isotropically consolidated sample using LS-DEM.

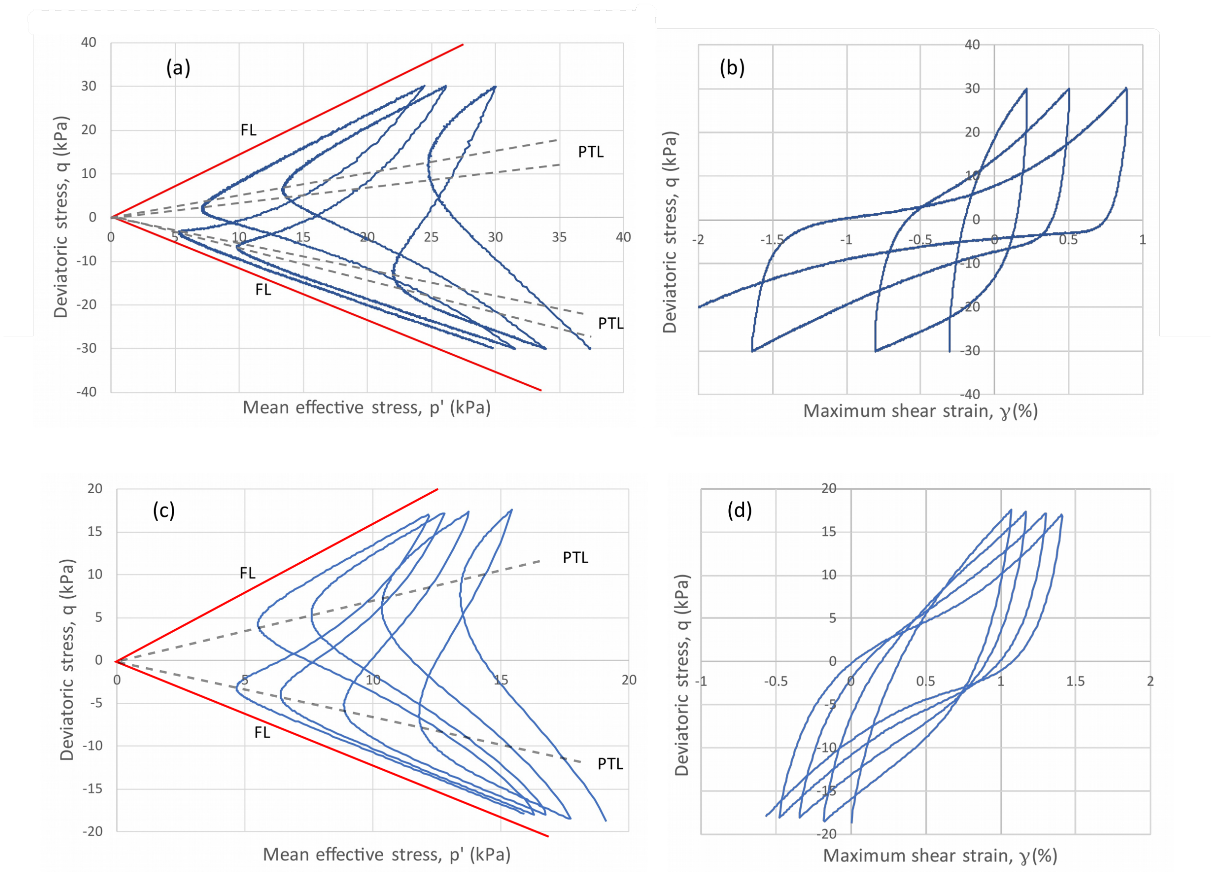

Figure 2.4 a) Cyclic undrained (constant volume) triaxial experiment on dense Karlsruhe sand (a and b), simulated test on Hostun sand (c and d) Stress path in p'-q stress space (a and c) and maximum shear strain versus deviatoric stress loops (b and d).

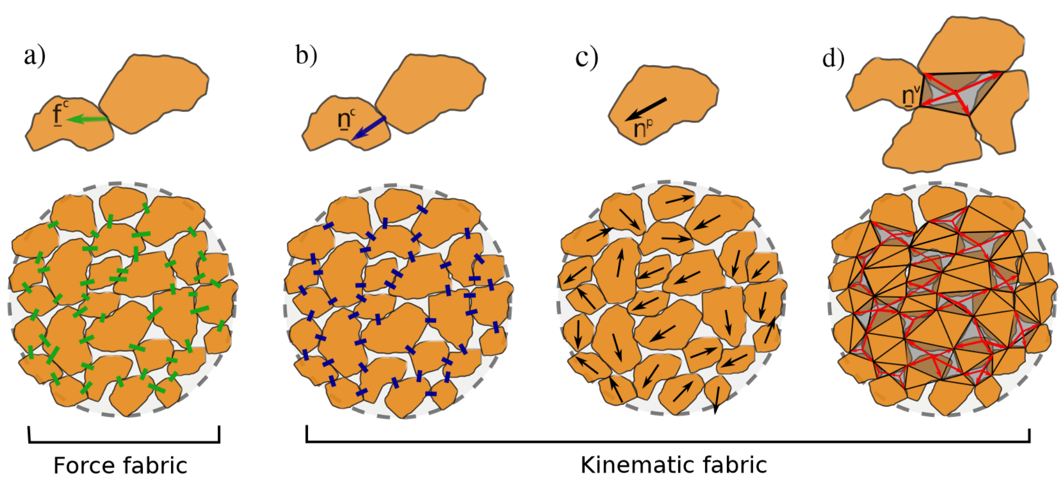

Figure 2.5 Examples of fabric descriptors: a) Contact forces, b) Contact normals, c) Particle long-axis, and d) Tesselation-based void vectors.

3 KEY OUTCOMES OF THE PROJECT

Main outcomes for this project can be analyzed in terms of monotonic (triaxial compression and extension simulations) and cyclic (different simulation setups) results.

3.1 MONOTONIC SIMULATION RESULTS

Simulation of monotonic loading conditions such as those by (Kawamoto et al. 2018), mentioned in the sections above, and additional testing carried out, showed the accuracy of LS-DEM in representing the behavior of granular assemblies. This is due to its use of realistic grain geometries and contact information with respect to the experimental samples used as input data. As Figure 1.2. showed, monotonic simulation and experimental results are very similar not only for global descriptors such as strain and stress, but also for micro quantities such as individual grain displacement and rotation, and the formation of localized phenomena such as shear banding.

Figure 3.1 and Figure 3.2 also show the importance of arbitrary shape in capturing realistic strain behavior and how the assumption of idealized spherical grains can result in significant differences when modeling granular materials. This outcome confirmed that LS-DEM was a reliable source of information for geomechanics modeling and could be used to developed virtual experiments with cyclic loading to obtain more information on fabric evolution.

3.2 CYCLIC SIMULATION RESULTS

A cylindrical sand sample was isotopically consolidated to 430 kPa and underwent triaxial compression and extension cycles. The triaxial cell was scanned using X-ray computed tomography to obtain 3D pictures of the individual sand grains, which were then converted to digital equivalents or avatars to be simulated in LS-DEM. The setup is shown below on Figure 3.3. for the triaxial sample with x-ray source. Figure 3.4. shows a stress-strain cyclic curve for the experiment and LS-DEM simulation. It is possible to observe that LS-DEM was also able to replicate expansion and compression loops characteristic of cyclic loading. Figure 3.5. shows how the simulation and experiments matched for different stages of compression and extension. It is important to mention that while the compression stage of the simulation matched very well with the experiment, the strain rate for the extension stage needs to be tuned carefully to avoid differences with experimental measures. Nevertheless, the capability of reproducing cyclic loading was also confirmed.

As an outcome of this project, simulations have been developed to use grains with arbitrary shapes obtained through CT scans of actual laboratory samples from the University of Grenoble, and subject them to cyclic loading conditions analog to those applicable via experiments, as a virtual laboratory. Initially, cycles have been applied in the range of a few dozens to a few hundreds, and evolution of cyclic descriptors over the application of these cycles has been studied. The ultimate objective could even be extrapolating how millions of low intensity cycles can end up modifying fabric descriptors and engineering quantities such as displacements and rotations, strengthening soils to resist extreme loading conditions.

To compare and extend the capabilities of existing experimental apparatuses, we also proposed new apparatuses or sample preparation methods in addition to true triaxial testing shown in the sections above. Some of the configurations considered so far for cyclic simulations included:

a.) Triaxial apparatus with flexible membrane (cyclic changes in confining pressure and vertical strain) (Figure 3.6 a.)

b.) Hollow Cylindrical Apparatus (HCA) with flexible membranes (shear cycles rotating lateral membranes) (Figure 3.6 b.)

c.) Hollow Cylindrical Apparatus (HCA) with rigid walls (shear cycles rotating lateral walls) (Figure 3.6 c.)

d.) Ring shear apparatus with rigid walls (shear cycles rotating horizontal walls) (Figure 3.6 d.)

Subjecting the different configurations to cycles with LS-DEM allowed to capture different properties, fabric tensor descriptors and other output that fluctuated accordingly to the cycles imposed. The most important aspect of this cyclic application was that, for some descriptors, a cumulative change developed with an increasing number of cycles. Figure 3.7 a.) shows the force chain distribution in three dimensions that is obtained from LS-DEM simulations and used to develop the different fabric tensors. Here only the contact normal fabric tensor (Figure 3.7. c.) and weighted force fabric tensor (Figure 3.7.d.) are presented since they show significant variation with cyclic loading, unlike an alignment tensor which did not behave the same, possibly due to the lack of elongated grains used for these simulations as the former two aspects wanted to be emphasized. Note that the contact normal tensor deviatoric component seems to increase over time, unlike the weighted force deviatoric component. Other quantities that indicate densification over time are void ratio (which decreases over cycles) and coordination number (which tends to increase with more cycles) as seen in Figure 3.7. b.). To show another way to visualize these changes in forces and contacts, Figure 3.8. displays how a three-dimensional polar histogram can be developed for the granular assembly to track changes on longitudinal/shear cycles and how this histogram tends to align force and contacts in the direction of the principal stress component.

CHAPTER 3: FIGURES

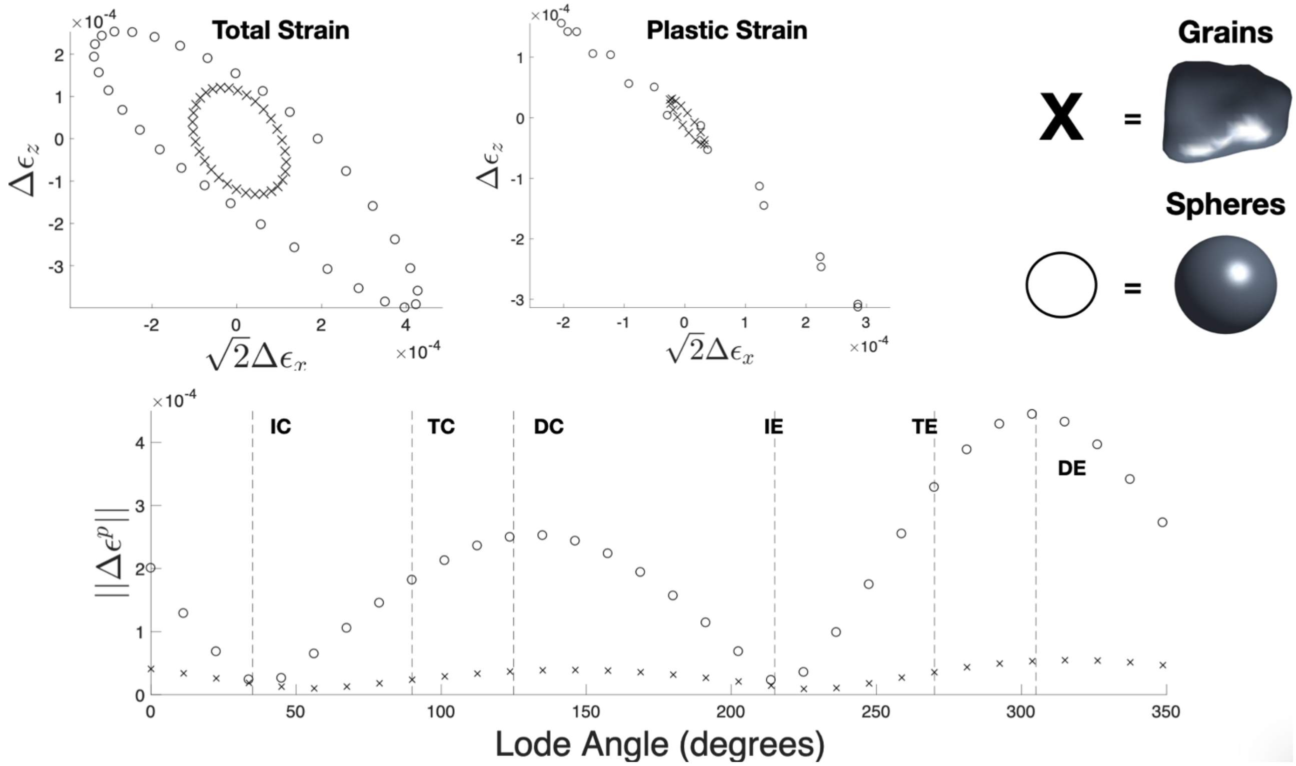

Figure 3.1 **Effect of shape on longitudinal versus transversal strains and lode angle.**

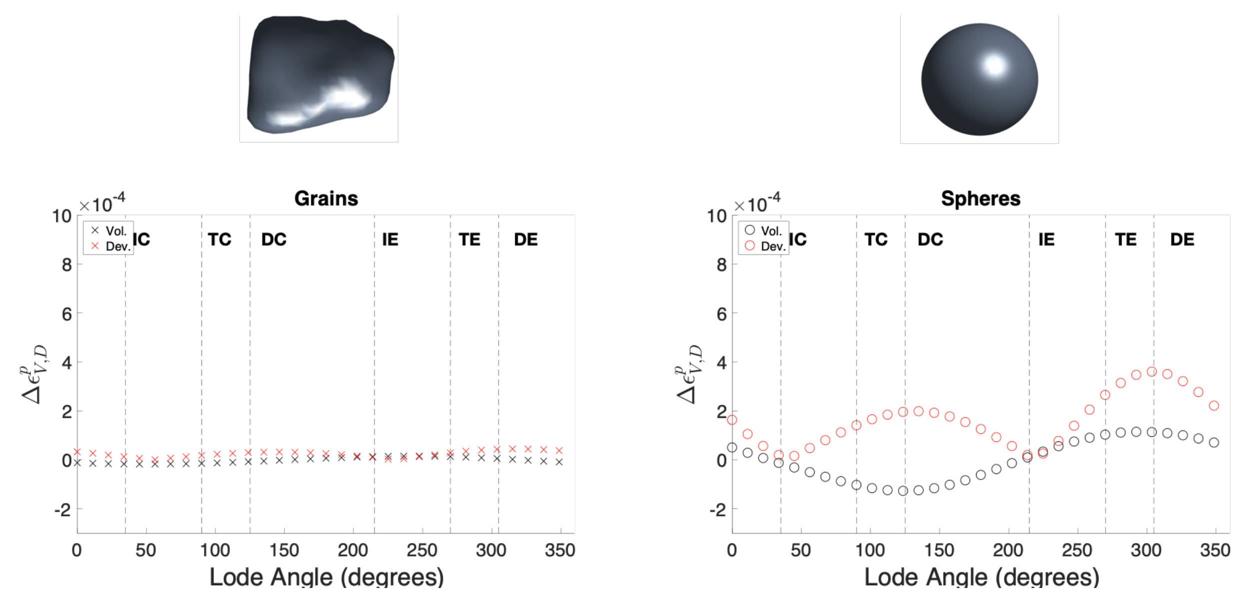

Figure 3.2 **Effect of shape on volumetric and deviatoric strains and lode angle.**

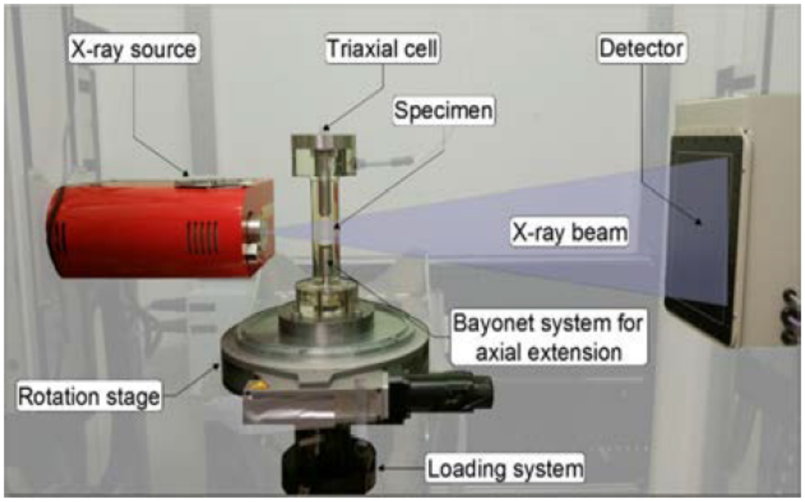

Figure 3.3 Triaxial sample setup for cyclic loading.

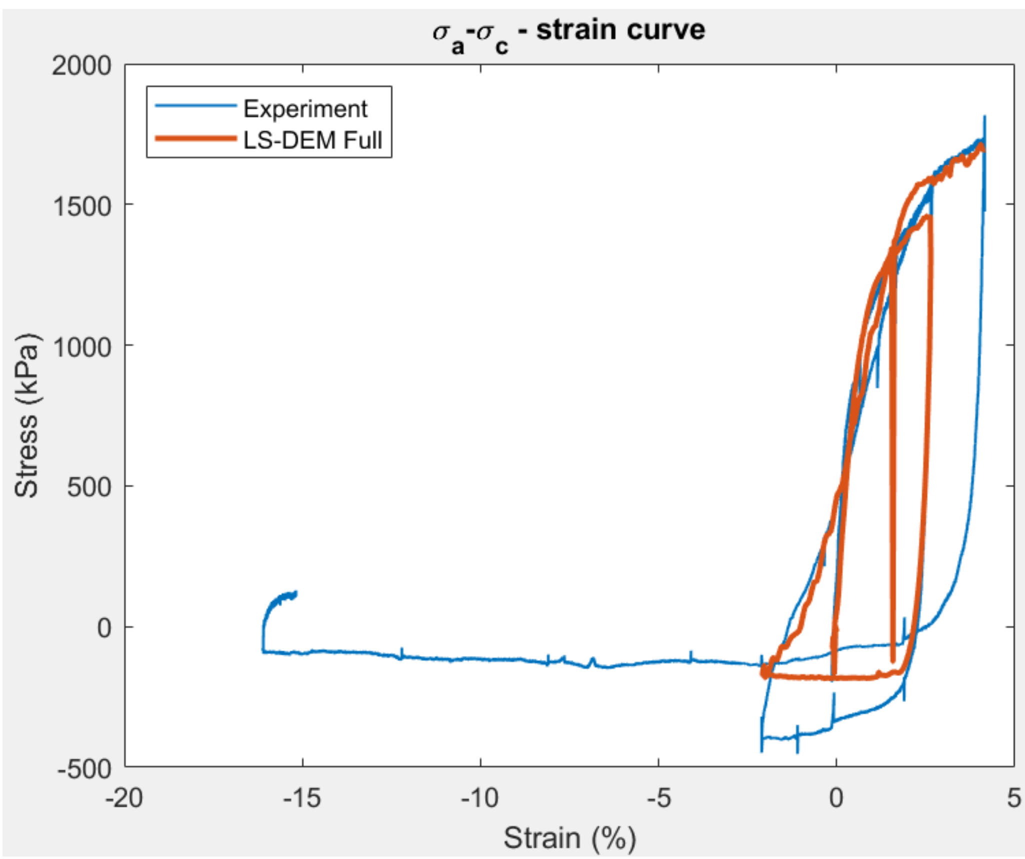

Figure 3.4 Comparison of Experiment and LS-DEM Simulation for Triaxial Cyclic Loading.

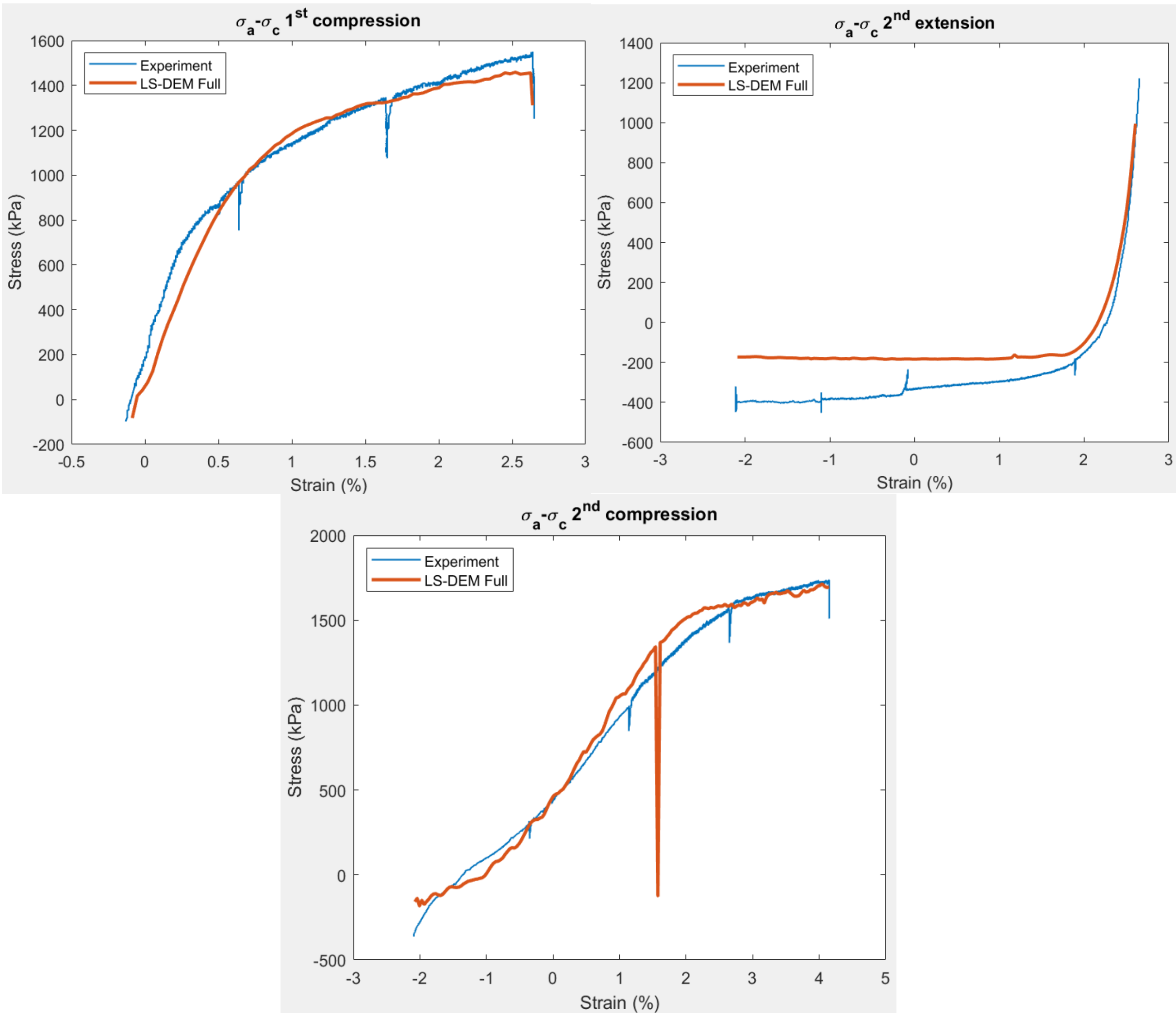

Figure 3.5 Comparison of stress-strain curves for different stages of the cyclic triaxial test.

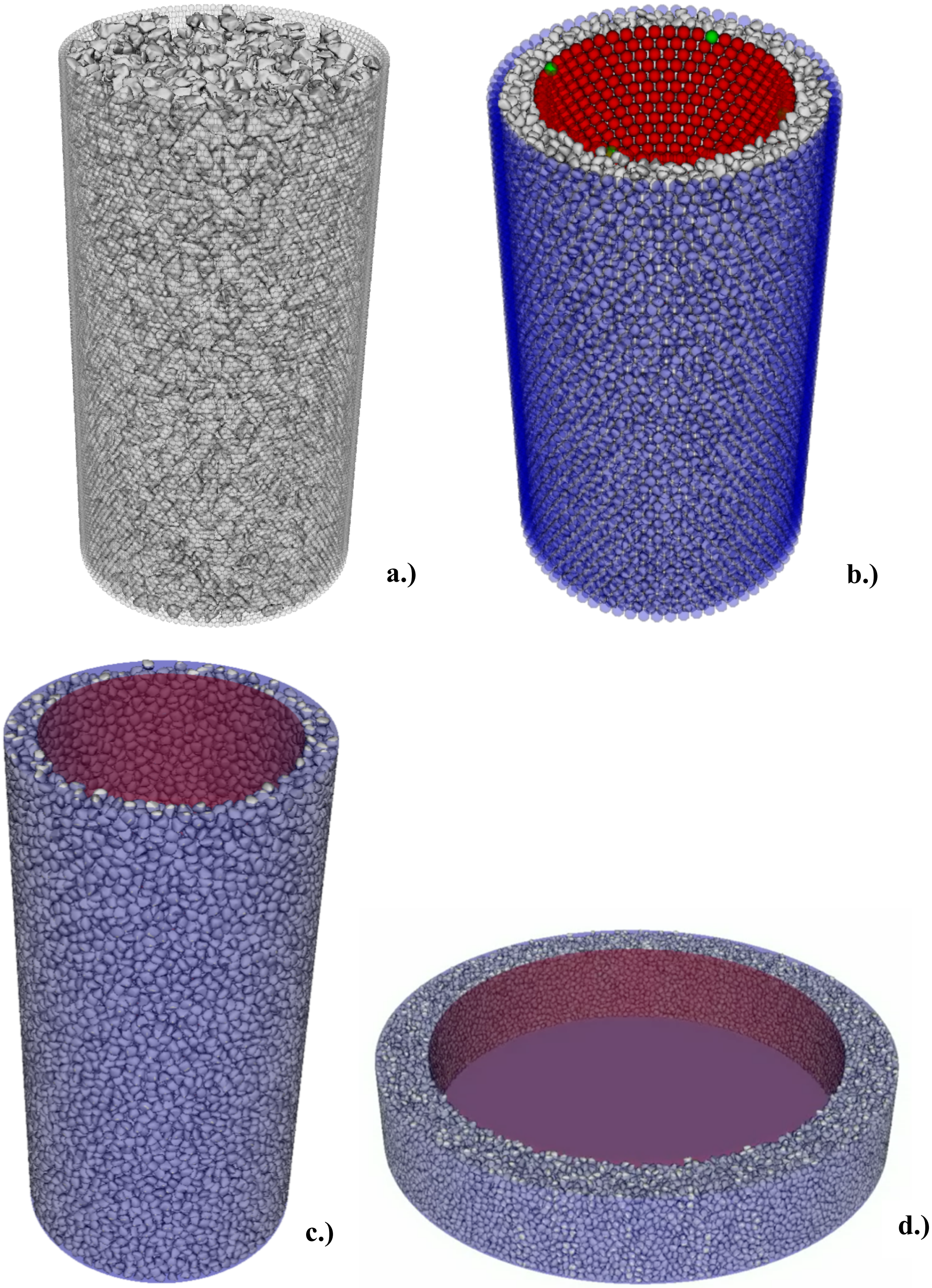

Figure 3.6 Different simulation configurations implemented: a.) Triaxial apparatus with flexible membrane b.) Hollow Cylindrical Apparatus (HCA) with flexible membranes c.) HCA with rigid walls d.) Ring shear apparatus.

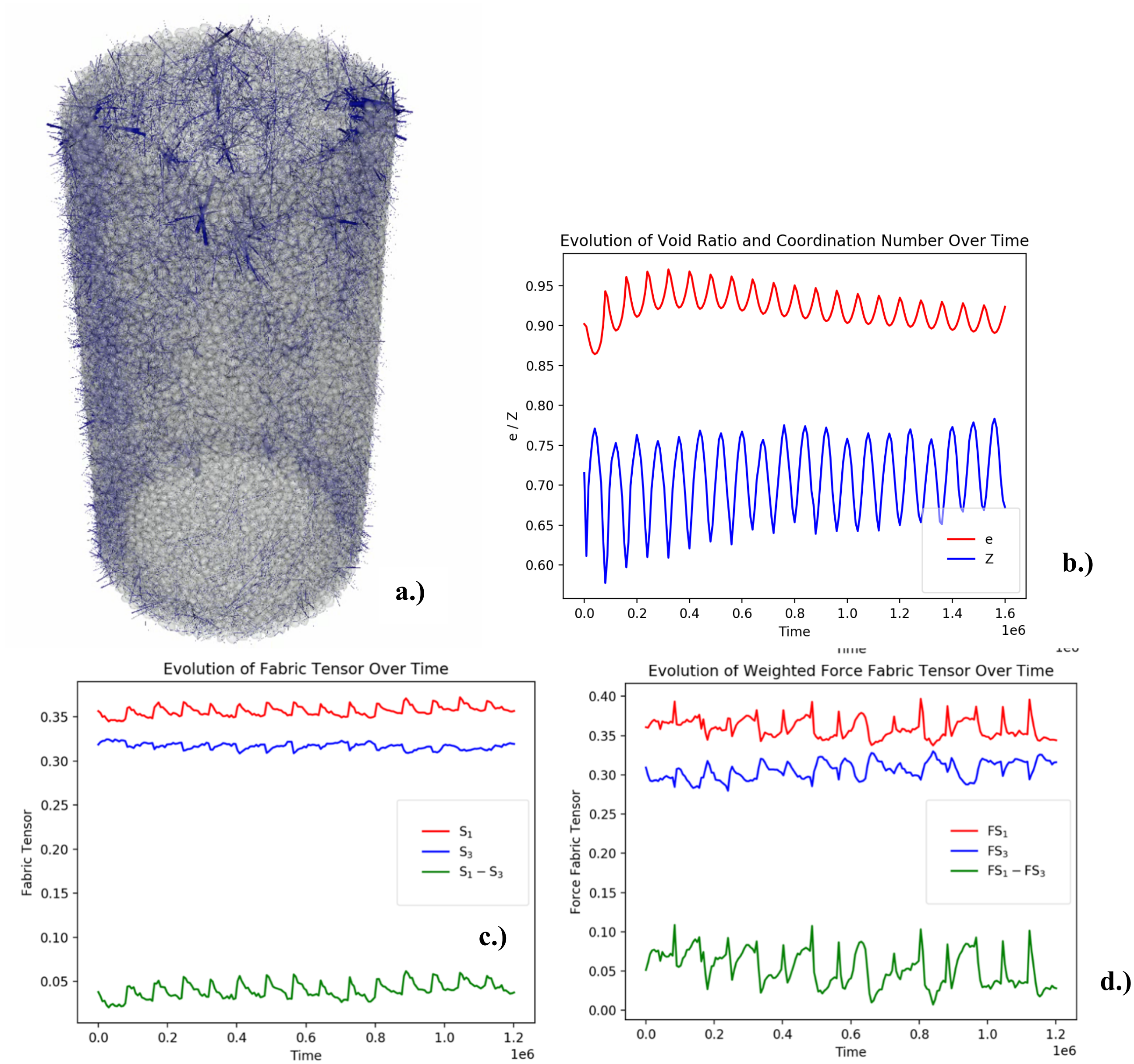

Figure 3.7 a.) Plot of intergranular contact and forces used to generate fabric tensors b.) Evolution of void ratio and coordination number c.) Evolution of principal components of normal contact fabric tensors and deviatoric component d.) Evolution of PCs of weighted force fabric tensor

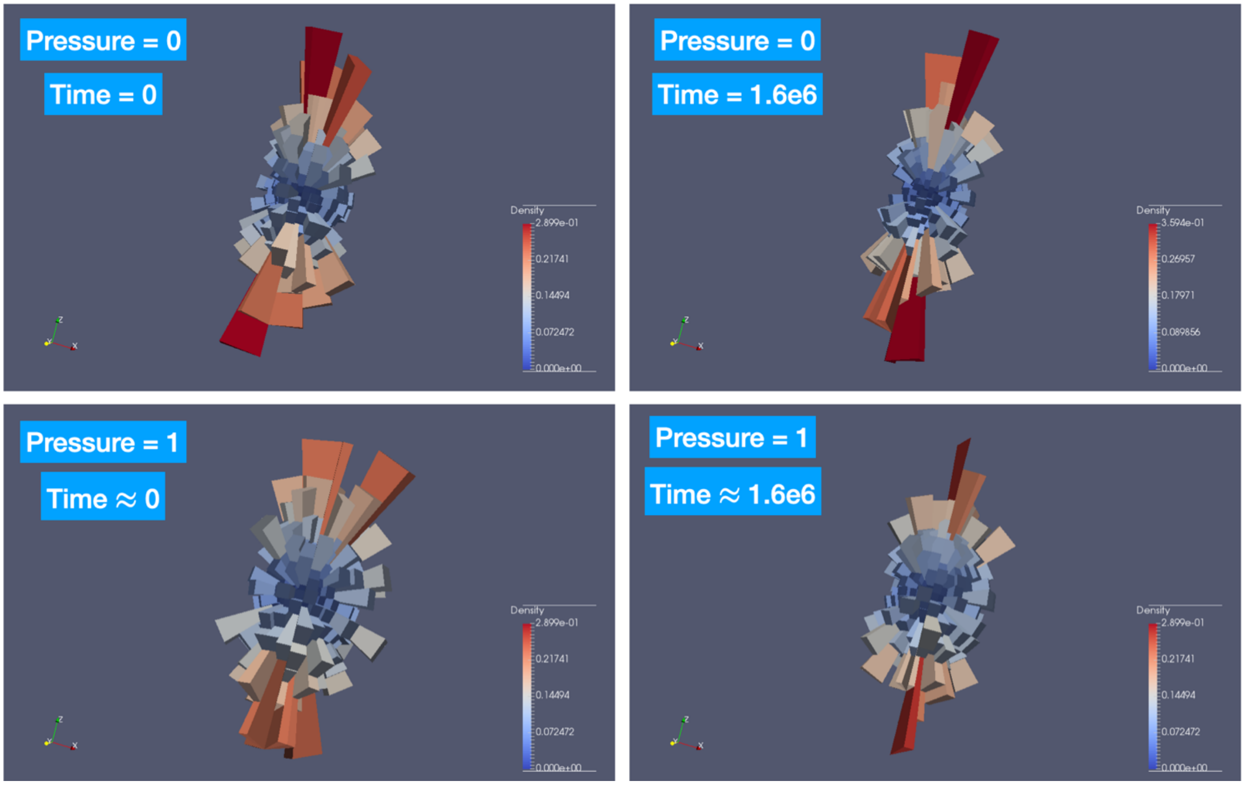

Figure 3.8 Variations in the polar histogram of contact and forces at different time and confining pressures.

4 CONCLUSIONS

4.1 SUMMARY

Summing up the most important highlights of the project we consider essential to mention:

1. LS-DEM can capture very accurately monotonic triaxial shear or compression experiments, matching stress and strain behavior from experiments and reflecting a better performance when using arbitrary-shaped digital avatar of experimental grains. In addition, this behavior also applies for cyclic triaxial loading conditions, either for longitudinal or shear testing. Nevertheless, cyclic loading requires a stricter control of boundary conditions in the simulation to avoid measurements errors and a larger number of computational resources given simulation time that permits a quasistatic regime for all cycles.

2. Even for a limited number of cycles, it is possible to observe cyclic evolution of fabric descriptors using LS-DEM. It provides unprecedented access to the full range of fabric descriptors, including the force fabric, which has not yet been investigated in real sands, due to limitations in existing techniques. Global quantities such as the coordination number and void ratio tend to oscillate over time but, in general, converge to different values in comparison to monotonic loading. We even observed this type of variation for the normal contact fabric tensor. This matches the existing knowledge on compaction and packing phenomena, where applying energy to a system causes re-accommodation of particles that alter granular behavior. The same happens for fabric descriptor tensors. Their principal components oscillate, however, if the fabric is significantly loose, they tend to keep converging (that is, their mean value between cycles) over time to new major and minor component values. This effect is expected to be augmented if the number of cycles and amplitude are increased.

3. The use of different experimental setups from the triaxial apparatus can provide different insight on the effect of boundary conditions and loading on fabric. Certain setups, such as true triaxial and cylindrical triaxial with flexible membrane simulations worked better to analyze extensional and compressional cycles; while others, such as rigid and flexible walls HCA, were better for observing cycles of shear and their effect on fabric descriptors.

4. There are indications that high frequency, low amplitude cycles have the potential to modify/densify a soil sample if subjected to enough loading. This pre-densification can aid in the performance of foundations and soils subjected to failure conditions and might significantly affect the limit loading they can

endure. This makes sense as this process of cyclic loading emulates the application of compaction on the granular material (for example, vibratory compaction).

5. Grain morphology, or attributes also play an important role, as more angular and elongated morphs have the tendency to amplify fabric effects. This is evident from the monotonic comparison presented previously, as grains that are like spheres show a different behavior than more irregular ones. In particular, the alignment tensor fabric descriptor did not show relevant cyclic changes for relatively spherical grains even if they had arbitrary shapes.

6. By leveraging virtual testing, the proposed research allows the attainment of stress paths and loading conditions, far beyond the experimentally accessible ones. This has the potential to motivate the design of new experimental apparatuses and inspire a new generation of predictive constitutive models. This research also lays the groundwork for follow-up research that goes beyond dry sands to include other complex factors that are present in natural granular systems. For example, sand deposits in nature are often affected by cementation due to aging and capillary adhesion due to partial saturation. The presence of clayey fines can increase the plasticity of sandy material and thermal expansion, and contraction cycles that can induce densification.

4.1.1 Recommendations

Based on the conclusions above, additional activities that have been identified as essential to implement to attain more insight on cyclic granular fabric include:

a.) Execute additional experiments with apparatuses other than the standard triaxial machine and for a greater number of cycles, to obtain high resolution X-ray computer tomography data that can be then used to improve the LS-DEM model to better capture cyclic changes on granular materials.

b.) Using the computational setups already developed, examine the effect of sample preparation (e.g., dry tamping, pluviation, etc.) and sample bedding angle on cyclic fabric evolution using DEM simulations to provide more information on fabric descriptor tensors.

c.) Combine information about contact normal and contact force tensors, as well as particle alignment and void tensors, from simulations and experimental results to develop a fabric descriptor that is representative of these experiments and can be used to predict granular fabric evolution via “virtual” experiments.

REFERENCES

Alonso-Marroquin F. and Herrmann H. J. (2004). Ratcheting of granular materials. *Phys. Rev. Lett.*, 92:054301. http://dx.doi.org/10.1103/PhysRevLett.92.054301

Andrade J. E., Ramos A. M., and Lizcano A. (2013). Criterion for flow liquefaction instability. *Acta Geotechnica*, 8(5):525–535. http://dx.doi.org/10.1007/s11440-013-0223-x

Andrade J. E., Lim K., Avila C. F., and Vlahinić I. (2012a). Granular element method for computational particle mechanics. *Computer Methods in Applied Mechanics and Engineering*, 241–244:262 – 274. http://dx.doi.org/10.1016/j.cma.2012.06.012

Andrade J. E., Vlahinić I., Lim K.-W., and Jerves A. (2012b). Multiscale 'tomography-to-′ simulation' framework for granular matter: the road ahead. *Géotechnique Letters*, 2(3):135–139.

Bolton M. D. (1986). The strength and dilatancy of sands. *Géotechnique*, 36(1):65–78. http://dx.doi.org/10.1680/geolett.12.00023

Borja R. I. and Andrade J. E. (2006). Critical state plasticity. part vi: Meso-scale finite element simulation of strain localization in discrete granular materials. *Computer Methods in Applied Mechanics and Engineering*, 195(37–40):5115 – 5140. John H. Argyris Memorial Issue. Part I. http://dx.doi.org/10.1016/j.cma.2005.08.020

Cundall P. A. and Strack O. D. L. (1979). A discrete numerical model for granular assemblies. *Géotechnique*, 29(1) :47–65. http://dx.doi.org/10.1680/geot.1979.29.1.47

Dafalias Y. F. and Manzari M. T. (2004). Simple plasticity sand model accounting for fabric change effects. *Journal of Engineering Mechanics*, 130(6):622–634. http://dx.doi.org/10.1061/(ASCE)0733-9399(2004)130:6(622)

Dai B., Yang J., Zhou C., and Luo X. (2016). DEM investigation on the effect of sample preparation on the shear behavior of granular soil. *Particuology*, 25:111 – 121. http://dx.doi.org/10.1016/j.partic.2015.03.010

David C., García-Rojo R., and Herrmann H. J. (2005). Hysteresis and creep in powders and grains. In *Powders and grains*. https://doi.org/10.1201/NOE0415383486

Dobry R., Powell D., Yokel F., and Ladd R. (1986). Liquefaction potential of saturated sand — the stiffness method. In *Proceedings of the seventh world conference on earthquake engineering, Istanbul, Turkey, vol. 3*.

Fu P. and Dafalias Y. (2011). Fabric evolution within shear bands of granular materials and its relation to critical state theory. *International Journal for Numerical and Analytical Methods in Geomechanics*, 35(18):1918–1948. http://dx.doi.org/10.1002/nag.988

Gao Z. and Zhao J. (2015). Constitutive modeling of anisotropic sand behavior in monotonic and cyclic loading. *Journal of Engineering Mechanics*, 141(8):04015017. http://dx.doi.org/10.1061/(ASCE)EM.1943-7889.0000907

Gao Z., Zhao J., Li X.-S., and Dafalias Y. (2014). A critical state sand plasticity model accounting for fabric evolution. *International Journal for Numerical and Analytical Methods in Geomechanics*, 38(4):370–390. http://dx.doi.org/10.1002/nag.2211

García-Rojo R. and Herrmann H. J. (2005). Shakedown of unbound granular material. *Granular Matter*, 7(2):109–118. http://dx.doi.org/10.1007/s10035-004-0186-6

Jefferies M. G. (1993). Nor-sand: a simple critical state model for sand. *Géotechnique*, 43(1):91–103. http://dx.doi.org/10.1680/geot.1993.43.1.91

Katzenbach R. and Festag G. (2004). Material behaviour of dry sand under cyclic loading. *Cyclic behavior of Soils and Liquefaction Phenomena*. http://dx.doi.org/10.1201/9781439833452.ch19

Kawamoto R., Andò E., Viggiani G., and Andrade J. E. (2018). All you need is shape: Predicting shear banding in sand with LS-DEM. *Journal of the Mechanics and Physics of Solids*, 111:375 – 392. http://dx.doi.org/10.1016/j.jmps.2017.10.003

Kawamoto R., Andò E., Viggiani G., and Andrade J. E. (2016). Level set discrete element method for three-dimensional computations with triaxial case study. *Journal of the Mechanics and Physics of Solids*, 91:1 – 13. http://dx.doi.org/10.1016/j.jmps.2016.02.021

Ladd R. (1974). Specimen preparation and liquefaction of sands. *Journal of the Geotechnical Engineering Division*, 100(10):1180–1184. http://dx.doi.org/10.1061/AJGEB6.0000117

Li X. S. and Dafalias Y. F. (2012). Anisotropic critical state theory: Role of fabric. *Journal of Engineering Mechanics*, 138(3):263–275. http://dx.doi.org/10.1061/(ASCE)EM.1943-7889.0000324

Li X. and Li X. (2009). Micro-macro quantification of the internal structure of granular materials. *Journal of Engineering Mechanics*, 135(7):641–656. http://dx.doi.org/10.1061/(ASCE)0733-9399(2009)135:7(641)

Mital U., Kawamoto R., and Andrade J. E. (2019). Effect of fabric on shear wave velocity in granular soils. *Acta Geotechnica*. http://dx.doi.org/10.1007/s11440-019-00766-1

Ng T.-T. (2009). Discrete element method simulations of the critical state of a granular material. *International Journal of Geomechanics*, 9(5):209–216. http://dx.doi.org/10.1061/(ASCE)1532-3641(2009)9:5(209)

Niemunis A., Wichtmann T., and Triantafyllidis T. (2005). A high-cycle accumulation model for sand. *Computers and Geotechnics*, 32(4):245 – 263. http://dx.doi.org/10.1016/j.compgeo.2005.03.002

Oda M. (1993). Inherent and induced anisotropy in plasticity theory of granular soils. *Mechanics of Materials*, 16(1):35 – 45. Special Issue on Mechanics of Granular Materials. http://dx.doi.org/10.1016/0167-6636(93)90025-M

Oda M. (1972). Initial fabrics and their relation to mechanical properties of granular materials. *Soils and Foundations*, 12(1):17–36. http://dx.doi.org/10.3208/sandf1960.12.17

Oda M., Konishi J. and Nemat-Nasser S. (1982). Experimental micromechanical evaluation of strength of granular materials: Effects of particle rolling. *Mechanics of Materials*, 1(4):269 – 283. http://dx.doi.org/10.1016/0167-6636(82)90027-8

Oda M. and Iwashita K. (1999). *Mechanics of granular materials: An introduction*. A.A. Balkena, Rotterdam, The Netherlands. http://dx.doi.org/10.1201/9781003077817

Radjai F., Troadec H., and Roux S. (2004). Key features of granular plasticity. In Antony S., Hoyle W., Ding Y., and Ding Y., editors, Granular Materials: Fundamentals and Applications, pages 157-184. The Royal Society of Chemistry. http://dx.doi.org/10.1039/9781847550996-00157

Satake M. (1982). Fabric tensor in granular materials. In Vermeer, P. A. and Luger, H. J., editors, *Proceedings of the IUTAM symposium on deformation and failure of granular materials*, pages 63–68. A.A. Balkem, Amsterdam.

Satake M. (1993). New formulation of graph-theoretical approach in the mechanics of granular materials. *Mechanics of Materials*, 16(1):65 – 72. http://dx.doi.org/10.1016/0167-6636(93)90028-P

Schofield M. and Wroth C. (1968). *Critical State of Soil Mechanics*. McGraw-Hill: London.

Sze H. Y. and Yang J. (2014). Failure modes of sand in undrained cyclic loading: Impact of sample preparation. *Journal of Geotechnical and Geoenvironmental Engineering*, 140(1):152–169. http://dx.doi.org/10.1061/(ASCE)GT.1943-5606.0000971

Tong Z., Fu P., Zhou S., and Dafalias Y. F. (2014). Experimental investigation of shear strength of sands with inherent fabric anisotropy. *Acta Geotechnica*, 9(2):257–275. http://dx.doi.org/10.1007/s11440-014-0303-6

Uchida A., Hatanaka M., and Taya U. (2001). Effect of anisotropy on drained and undrained shear behavior of in-situ sandy soils. *Proceedings of the International Conference on Recent Advances in Geotechnical Earthquake Engineering and Soil Dynamics*. http://dx.doi.org/10.1201/NOE9058096043.ch66

Vaid Y. and Chern J. (1983). Effect of static shear on resistance to liquefaction. *Soils and Foundations*, 23(1):47–60. http://dx.doi.org/10.3208/sandf1972.23.47

Vaid Y., Sivathayalan S., and Stedman D. (1999). Influence of specimen-reconstituting method on the undrained response of sand. *Geotechnical Testing Journal*, 22(3):187–195. https://doi.org/10.1520/GTJ11110J

Vlahinić I., Andò E., Viggiani G., and Andrade J. (2014). Towards a more accurate characterization of granular media: extracting quantitative descriptors from tomographic images. *Granular Matter*, 16(1):9–21. http://dx.doi.org/10.1007/s10035-013-0460-6

Vlahinić I., Thomas J. J., Jennings H. M., and Andrade J. E. (2012). Transient creep effects and the lubricating power of water in materials ranging from paper to concrete and kevlar. *Journal of the Mechanics and Physics of Solids*, 60(7):1350 – 1362. http://dx.doi.org/10.1016/j.jmps.2012.03.003

Wang R., Fu P., Zhang J.-M., and Dafalias Y. (2017). Evolution of various fabric tensors for granular media toward the critical state. *Journal of Engineering Mechanics*, 143(10):04017117. http://dx.doi.org/10.1061/(ASCE)EM.1943-7889.0001342

Wichtmann T. and Triantafyllidis T. (2016a). An experimental database for the development, calibration and verification of constitutive models for sand with focus to cyclic loading: part i—tests with monotonic loading and stress cycles. *Acta Geotechnica*, 11(4):739–761. http://dx.doi.org/10.1007/s11440-015-0402-z

Wichtmann T. and Triantafyllidis T. (2016b). An experimental database for the development, calibration and verification of constitutive models for sand with focus to cyclic loading: part ii—tests with strain cycles and combined loading. *Acta Geotechnica*, 11(4):763–774. http://dx.doi.org/10.1007/s11440-015-0412-x

Wichtmann T. and Triantafyllidis T. (2017). Strain accumulation due to packages of cycles with varying amplitude and/or average stress – on the bundling of cycles and the loss of the cyclic preloading memory. *Soil Dynamics and Earthquake Engineering*, 101:250 – 263. http://dx.doi.org/10.1016/j.soildyn.2017.07.012

Yamashita S. and Toki S. (1993). Effects of fabric anisotropy of sand on cyclic undrained triaxial and torsional strengths. *Solids and Foundations*, 33(3):92–104. http://dx.doi.org/10.3208/sandf1972.33.3_92

Yang Z. X., Li X. S., and Yang J. (2008). Quantifying and modelling fabric anisotropy of granular soils. *Géotechnique*, 58(4):237–248. http://dx.doi.org/10.1680/geot.2008.58.4.237

Yoshimine M., Ishihara K., and Vargas W. (1998). Effects of principal stress direction and intermediate principal stress on undrained shear behaviour of sand. *Soils and Foundations*, 38(3):179–188. https://doi.org/10.3208/sandf.38.3_179

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ISSN 2770-8314
https://doi.org/10.55461/RILY6540