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Virtual reality testing for more reliable design in sand

Essais en réalité virtuelle pour un dimensionnement plus fiable dans les sables.

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ABSTRACT: Current practice in geotechnical engineering uses physical laboratory testing to characterise the mechanical behaviour of soils. Laboratory tests, though necessary and useful, present several limitations, especially for the testing of granular soils. Most often the tests cannot be conducted on soil specimens that have the same conditions as in situ, nor in sufficient number to define all the material parameters needed in advanced constitutive models. Virtual Reality (VR) testing is emerging as a novel and efficient alternative that overcome some of the limitations and uncertainties from standard laboratory testing, and could revolutionise the state-of-the-art for characterising and modelling sand behaviour. This paper describes a framework to develop VR testing to a level where it can complement and perhaps substitute physical laboratory testing. The new approach is made possible by leveraging recent developments in Discrete Element Method (DEM), X-ray technology, image processing and high-performance computing. The paper also highlights the benefits of virtual testing for application in geotechnical engineering. The range of applications is infinite, and it could help address today's challenges, e.g., of safe tailings dams and cost-effective foundations for offshore wind turbines.

RÉSUMÉ : Aujourd'hui, la géotechnique utilise des essais en laboratoire pour caractériser le comportement du sable. Les essais de laboratoire présentent plusieurs limitations, en particulier pour les sols granulaires. Le plus souvent, les essais ne peuvent pas être menés sur des échantillons ayant les mêmes conditions qu'*in situ*, ni en nombre suffisant pour définir les paramètres nécessaires pour les modèles constitutifs avancés. Les essais en réalité virtuelle (VR) présentent une alternative efficace qui, non seulement pourra surmonter certaines des limitations et incertitudes des essais de laboratoire, mais aussi révolutionner l'état de l'art pour caractériser et modéliser le comportement des sables. L'article décrit une approche pour développer les essais VR qui pourront complémenter er remplacer nombre d'essais physiques en laboratoire. L'approche VR est rendue possible grâce aux développements récents de la méthode des éléments discrets, la tomographie et le calcul haute performance. La gamme d'applications est infinie et pourra aider à relever les défis actuels d'aujourd'hui par exemple en matière de barrages de résidus miniers et de fondations pour les éoliennes.

KEYWORDS: Virtual testing, Sand Characterisation, Sand modelling, Discrete Element Method, Foundation Design.

1 INTRODUCTION

Much of the world's buildings and infrastructure such as roads, railways, containment facilities and onshore- and offshore-energy installations, are founded on granular materials, most often sand. The design and safe operation of these structures require a fundamental understanding of sand behaviour and reliable constitutive models that can predict the deformations and strength of the sand for various loading conditions. Usually, such models treat the sand as a continuum, and their mathematical formulation is based on a relationship between effective stress and average deformation (strain) of a large assembly of grains in the sand. Despite extensive efforts to derive reliable predictive formulations, e.g. Liu et al. (2019) and Petalas et al. (2019) – just to mention two very recent contributions – there still does not exist a model that can predict the stress-strain behaviour of sands, especially when subjected to time-varying cyclic loading due to wind, waves, ice, or earthquakes (Jostad et al. 2020).

The inability of continuum models to correctly predict the behaviour of sand can be attributed to the fact that they are most often derived from observed behaviour on the continuum scale, without explicitly considering sand mechanics at the grain scale. Because the continuum models are phenomenological models, they tend to grow in complexity the more general they get. This results in models with many parameters that typically require extensive laboratory testing to calibrate them.

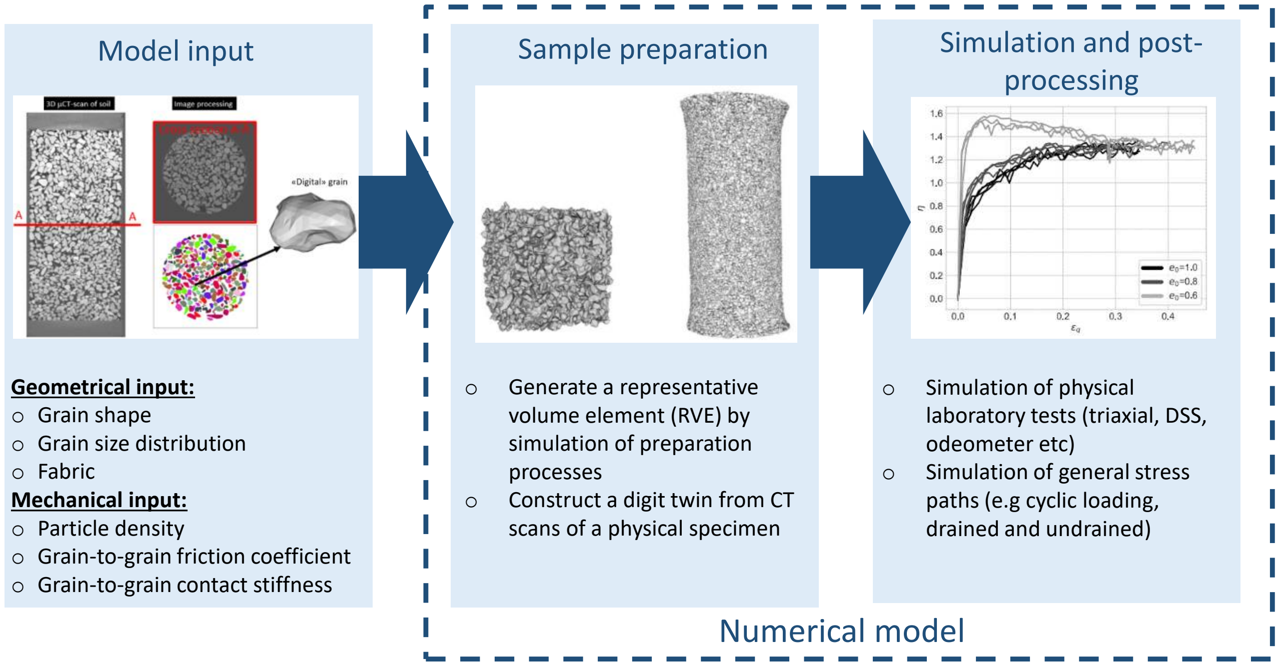
Current practice in geotechnical engineering most often uses physical laboratory tests to characterise the behaviour of sand. Laboratory testing presents important limitations, especially for testing sand at the same conditions as in situ, and it is practically and economically impossible to run enough laboratory tests to cover the spectrum of stress conditions of interest for a design.

Faced with the challenges posed by the representativeness of the sand tested in the laboratory and the reliability of the parameters for sand in models and design, there is ground to raise the following questions: i) could laboratory testing of sand be supplemented and perhaps replaced by numerical simulations, and ii) what are the possible benefits of this approach?

The present paper proposes a framework to develop Virtual Reality (VR) testing to supplement today's standard laboratory testing, based on novel developments within micromechanics of granular materials (Section 2) and highlights some of the benefits of VR testing in geotechnical engineering (Section 3).

2 VIRTUAL REALITY TESTING

The overall idea of VR testing of sand is to supplement and substitute today's standard laboratory tests on sand with a numerical simulation tool of digitised grains. The key components in the proposed framework are: 1) a particle-based numerical method, 2) a methodology to determine the input parameters to the numerical model, 3) a methodology for the preparation of the virtual specimen; and 4) simulation of the virtual laboratory tests and post-processing. Figure 1 presents schematically the steps in the proposed framework, and each of these components is explained in the following sub-sections.



Geometrical input:
- Grain shape
- Grain size distribution
- Fabric

Mechanical input:
- Particle density
- Grain-to-grain friction coefficient
- Grain-to-grain contact stiffness

- Generate a representative volume element (RVE) by simulation of preparation processes
- Construct a digit twin from CT scans of a physical specimen

- Simulation of physical laboratory tests (triaxial, DSS, odeometer etc)
- Simulation of general stress paths (e.g cyclic loading, drained and undrained)

Figure 1. Proposed framework for VR testing. The figure showing the triaxial test specimen (digital twin) is from Kawamoto et al. 2018.

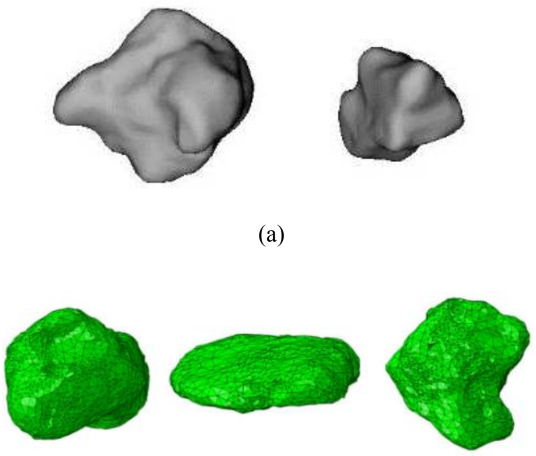
2.1 *Particle-based numerical method*

The simulation tool must be capable of modelling the fundamental mechanics of sand. Sand grain interaction depends on characteristics such as mineralogy, shape, angularity, roughness, and structure of the grain skeleton (fabric), together with the actual stress and stress history (Rowe 1962, Brewer 1964). These interactions define the contact forces between the grains and the pattern of relative displacements and rotations of the grains that cause the complex deformational response observed in sands (stiffness, strength, dilatancy, and strain accumulation).

One promising code for modelling the fundamental mechanics of sand is the *Level Set Discrete Element Method* (LS-DEM) developed by Kawamoto et al. (2016). LS-DEM is a three-dimensional DEM code that can simulate assemblies of particles of arbitrary shape using Level-Set (LS) functions (Fig 2a). A linear contact model and a Coulomb friction model are used for computing the normal and tangential forces between grains, however it is also possible to use other formulations if needed. These models can be simply described with virtual springs or more sophisticatedly by combination of virtual springs, sliders and dashpots with various complexities. LS-DEM has been validated by comparing results from a miniature triaxial compression test on HN31 Hostun sand performed inside an x-ray tomograph at Laboratoire 3SR in Grenoble (Kawamoto et al. 2018). A comparison on grain level was possible by comparing the simulations with tomographic images of the specimen at different stages in the test. The validation showed that the model is capable of reproducing both stress-strain behaviour and micro-scale behaviour (displacements and rotation of grains) even in the unstable post-peak regime with strain localisation. Jostad et al. (2021) also showed that the code can qualitatively model the behaviour of sand under cyclic loading, capturing features like strain accumulation and phase transformation from contractive to dilative behaviour during undrained cycles.

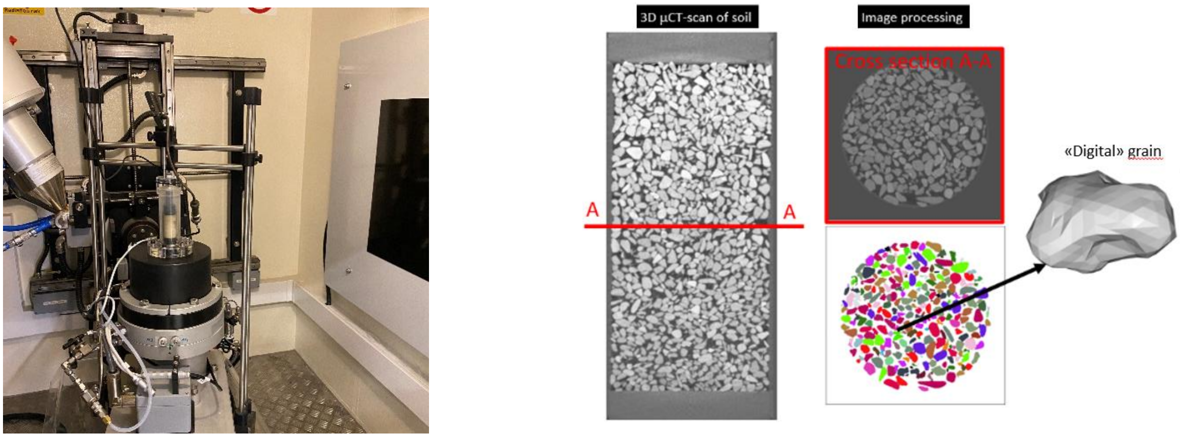
Another possible approach is to use a framework of combined discrete-finite-element method, such as the *"micro" finite element model* by Nadimi & Fonseca (2018). Here each grain is represented as a continuum deformable body and the interaction between grains results from deformation of these contacting bodies. The method allows for realistic representation of grain shape obtained from x-ray tomography (Fig 2b). In addition, the approach allows for modelling grain deformations and can provide insight about stress distribution and yielding within the grains. The micro-FE approach has been validated for the case of a triaxial test (Nadimi et al. 2020). The method is mostly relevant for problems where grain deformation is important for the material behaviour, e.g., particle yield or breakage, or for studying particle contact.

The main feature of both methods described above is the realistic representation of grain shape. For problems where grain shape is of less importance, e.g., for soils consisting of well-rounded grains, a regular DEM code with simplified particle shapes (spherical, elliptical or clusters of particles) may also be used for virtual testing, both for simplifying the model and for reducing computational time.


(a)

(b)

Figure 2. Realistic representation of grain shape in (a) LS-DEM (Kawamoto et al. 2016), (b) micro finite element model (Nadimi & Fonseca (2018).



(a) (b)

Figure 3. (a) X-ray tomograph with transparent triaxial cell on a rotating table. (b) Tomographic image processing .

2.2 *Method for determining input to the numerical model*

The inputs to the numerical model can be separated into geometrical and mechanical quantities. The geometrical input consists of the shape and size of individual grains and particle's mutual arrangement (fabric). The mechanical input depends on the numerical method. For DEM this is the grain density, grain-to-grain friction coefficient and grain-to-grain normal and tangential stiffness. The micro finite element method needs in addition parameter(s) to describe the grain stiffness. The number of parameters then depends on the chosen constitutive model - the simplest being an elastic modulus.

Two different approaches to determine the input parameters are presented here, using LS-DEM as an example. The first approach requires a physical experiment (a triaxial test) performed in a x-ray tomograph to calibrate an LS-DEM avatar model of the experiment ("digital twin") as shown in Kawamoto et al. (2018). The second method proposes a procedure where the input is determined without the need of a micro experiment performed inside the x-ray tomograph.

2.2.1 *Input determined from a digital twin*

The input parameters can be determined by numerical simulation of a digital twin, here referring to a numerical copy of a physical specimen. To create a digital twin it is necessary to identify the individual grains, their shapes and their positions from the physical specimen at the start of the test. This information makes up the geometrical input to the model. Further, the macro response (stresses and strains) and the pattern of individual grain displacements and rotations during the test should be recorded and used to compare with the simulations to calibrate the mechanical input parameters, i.e., the grain friction and contact stiffnesses are calibrated to match the behaviour obtained from the experiment.

The grain-scale information needed for this calibration can be achieved by use of a element testing device installed inside an x-ray tomograph. The present maximum number of grains that can be used in the numerical model is 50.000 - 100.000 and thus the dimensions of a sand specimen need to be significantly smaller than in a standard laboratory test. To obtain images throughout the test, the test is stopped and scanned at different stages. This involves stopping the test while maintaining the cell pressure constant and avoiding any movements of the soil during a scan. Testing is then resumed until the next scan takes place. Figure 3a shows a photograph of a triaxial cell with x-ray tomograph and detector panel. After the test is completed, the images are post processed using dedicated software, for instance SPAM (Stamati et al. 2020), and level set imaging algorithms (Vlahinic et al. 2014) to identify 3D particles and create a digital twin for the simulation (Fig. 3b).

Several challenges arise in this calibration process: (i) the use of specialized equipment and very small soil specimens (for instance 10mm in diameter, depending on the soil D50, resolution and testing purpose), (ii) the tomographic image acquisition that can introduce artefacts (blur, noise, rings, sharpness issues) and relaxation since the test needs to be stopped during scanning, (iii) spatial resolutions issues, related to the voxel size and the derived quantities, such as particle rotations and the identification of contacts, (iv) limitations on the particle sizes that can be identified, (v) complex boundary conditions (membranes, load and bearing plates) which needs to be modelled in the simulation, and (vi) time consuming processing. This method is therefore considered to be mostly useful for research studies, e.g., on less known materials (such as carbonates, glauconite etc,) or for validation exercises.

2.2.2 *Input determined without micro x-ray experiment*

As an alternative to calibrating the input parameter against the results of a micro experiment performed inside an x-ray tomograph, the input parameters can be estimated from less advanced tests. The approach is based on the assumed premise that grain shape and contact friction are the most important parameters to describe soil behaviour, and that the contact stiffness can be given as numerical value that will result in a realistic response, and at the same time does not cause numerical convergence or too long calculation time.

The grain shapes are still obtained from x-ray tomographic images, but rather than scanning a specimen inside a triaxial cell, this can be done by scanning a representative selection of grains – not assembled - to enhance the resolution and avoid particle contacts that may affect the identification of particles during the image processing.

The internal friction coefficient can be determined by calibration to a simple physical experiment like the fixed funnel method (Beakawi Al-Hashemi & Baghabra Al-Amoudi 2018), normally used to find the angle of repose. The calibration is done by tuning the friction coefficient in a numerical simulation of the experiment until achieving the same angle of repose as measured in the experiment.

With time a library of virtual grains and DEM input parameters for various sands will gradually be developed, allowing for more efficient virtual testing with less time needed for model calibration.

2.3 *Preparation of virtual specimen*

The digital specimen must be packed to a certain initial state, as it is also the case for physical experiments performed in the laboratory. This is a crucial part of the modelling since it determines the initial stress state and the initial fabric of the sample, meaning the void ratio, the particle orientations and the particle contacts.

The initial state of the specimen may be constructed from tomographic images of a physical experiment, either as a full "digital twin" where also the experimental boundary conditions such as membranes and load and bearing plates are modelled (as shown in Kawamoto et al. 2018), or by extracting a sub-model of the physical specimen as a "representative volume element" (RVE).

More generally, the initial state may be generated by simulating a specimen preparation process. Agnolin and Roux (2007) presents various assembling processes and investigate the influence of the assembling process on the microstructure of the packing. One method is to assemble the grains in a gas state and compact it. An example of a grain assembly prepared from a gas state in LS-DEM is shown in Figure 4. Other methods aim at simulating traditional procedures used in soil testing, such as pluviation ("rain" deposition under gravity) or vibration. Karapiperis et al. (2021) presents a preparation technique where grains are pluviated into a container, using LS-DEM. By simulating different preparation techniques and varying parameters such as the initial particle orientation, grain friction and damping, a range of initial fabric can be simulated.

Figure 4. View of a virtual true triaxial specimen with periodic boundaries in LS-DEM, prepared by compacting the grains from a gas state.

2.4 *Simulation of laboratory tests and post-processing*

By using mixed boundary conditions, loads and deformations can be applied to the digital specimens/virtual samples to simulate idealized stress and strain paths (similar to physical laboratory tests such as triaxial, direct simple shear (DSS) or oedometer tests), as well as investigate any other complex testing conditions (principal stress rotations, irregular cyclic loading etc). During the simulation, the macro response of the material in terms of stresses and strains is computed. In addition to stress-strain response, micro scale information such as the evolution of contact forces, the particle and contact orientations, the particle displacements and rotations, etc. can be computed and post-processed.

As an example of the use of virtual testing, results from LS-DEM simulations were used to establish the input parameters to the Sanisand constitutive model of Taiebat and Dafalias (2008) for an angular sand. The Sanisand model is a stress-ratio controlled constitutive model based on elasto-plasticity and critical state theory. Several versions with different features exist within the Sanisand model family, and each require 15 to 20 input parameters. To determine the input parameters, a series of triaxial compression tests with various initial void ratio and confining pressure were simulated with LS-DEM. The stress-strain response from the simulations were used to determine the critical state parameters and the elastic stiffness, dilatancy and kinematic hardening parameters in the Sanisand model. Figure 5 gives an example of some of the test results in terms of stress-strain curves and the resulting Sanisand model constant n_b controlling peak friction angle. The same preparation method was used for all simulations, which means that the initial fabric in the VR testing was more repeatable than in the laboratory. The model constants obtained would then be more consistent than from laboratory tests.

Figure 5 shows another example of where LS-DEM was used to simulate the stress-strain response of an undrained cyclic triaxial test on Hostun sand (Jostad et al. 2021). The response displays the main characteristics of a real test, such as cyclic strain accumulation and phase transformation between contractive and dilative behaviour within stress cycles.

3 BENEFITS OF VIRTUAL REALITY TESTING

VR-testing can become a powerful and, with time, proven tool that engineers and researchers will use and build upon to both solve geotechnical engineering problems and move the boundaries of scientific knowledge.

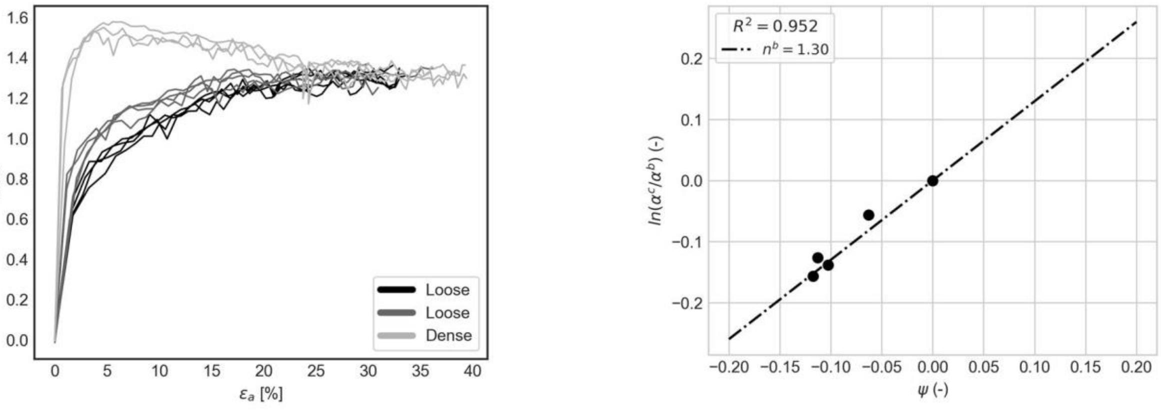


Figure 5. LS-DEM simulation of drained triaxial tests to determine input parameters in the Sanisand model. Left: Stress ratio q/p' vs deviatoric strain; Right: Curve-fitting of the model constant n_b controlling the peak friction angle.

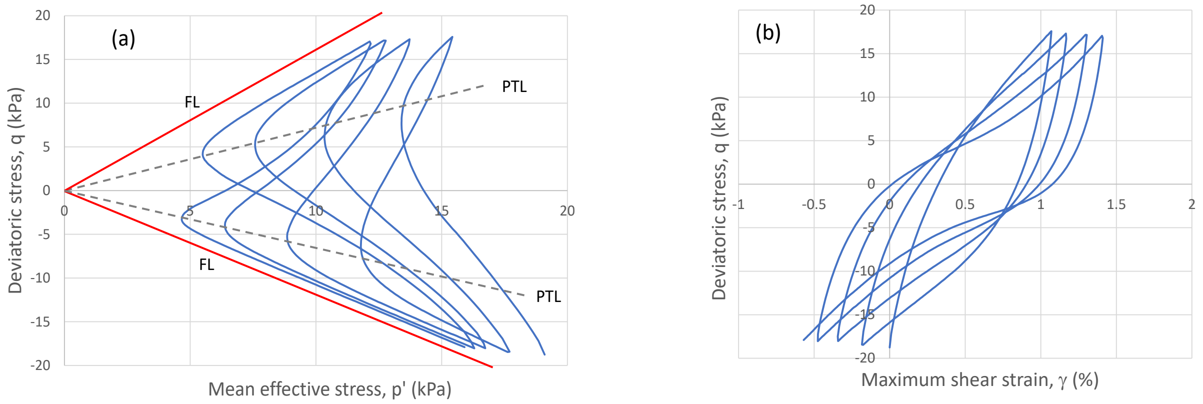


Figure 6. LS-DEM simulated cyclic undrained (constant volume) triaxial test on Hostun sand: (a) stress path in p'-q stress space; (b) maximum shear strain versus deviatoric stress loops (modified after Jostad et al. 2021)

In particular, VR-testing is expected to bring the following new developments and new benefits:

1. *Reduce limitations and uncertainties in the behaviour of sand from standard laboratory testing.* Examples of uncertainties are non-uniform deformations within the test specimens (Desrues et al. 2018), which may be caused by boundary effects in the test set-up, varying initial fabric during specimen preparation, and test repeatability and reliability. VR-testing will allow quantifying the effect of the specimen preparation method and identify the sample's deformation characteristics.
2. *Allow a large number of tests to be run to ascertain behaviour and the parameters to use for design.* This will be beneficial for calibration of advanced constitutive models requiring many calibration tests.
3. *Scale up laboratory testing*. VR-testing will allow testing of granular materials whose particles are too large for standard laboratory equipment, e.g., track ballast for railways and scour protection for offshore installations.
4. *Investigate all types of loading and deformation histories*, which cannot be achieved with existing conventional testing apparatus. The response of sand to irregular cyclic load histories has not been systematically tested, and its behaviour under non-standard stress systems is far from fully understood. This knowledge gap prevents the development of reliable constitutive models that can be used in design. The relationship between sand fabric and accumulated deformations is not well understood today (Jostad et al. 2020), and it is not possible to model it accurately. VR testing will allow to run tests under general loading, including monotonic, radial, cyclic, and multi-directional tests, and any loads inducing principal stress axis rotation.

   The findings from VR testing will impact research for all types of civil engineering constructions. This is particularly relevant for (1) offshore wind turbines because of the complex stress paths around monopiles that need to be simulated; (2) slopes where shearing in different directions needs to be investigated in stability analyses; and (3) when the response of a sand depends on the degree of drainage taking place in the foundation.
5. *Explore the influence of fabric on the behaviour of the sand.* Achieving an improved grasp of the role of fabric will lead to an understanding of the physical mechanisms controlling accumulation of strains in sand, as well as the incidence of liquefaction and liquefaction potential in sands. These aspects are essential challenges for developing solutions for offshore wind farms, earthquake engineering and the stability (or danger of instability) of tailings dams on the short and long term.
6. *Facilitate the establishment of robust relationships for sands.* The authors believe that the basic properties of sand (mineralogy, grain size distribution, shape, angularity, void ratio) and fabric can be related to the complex stress-strain history and stress-path dependent deformation response of the sand (non-linear behaviour, dilatancy and strength), and that the relationships can be generalised to cover different types of sands.

   These relationships thus developed may be used by (1) the research community to further develop constitutive models and (2) practitioners to fill in data and behavioural gaps for infrastructure projects (e.g., while planning site investigations) or to help control the results of laboratory tests.
7. *Contribute and accelerate machine learning-based research*. Machine learning (ML) has emerged as a powerful technique to calibrate constitutive sand models, but no useful formulations have yet been established due to insufficient data. VR-testing, by producing a lot of tests very efficiently, will provide large volumes of quality data suitable for ML. By mixing digitised sands with different grain shapes and angularities a large range of virtual sand specimens with varying index properties can be simulated. The data sets can further be fed into a Deep Learning (DL) framework to develop improved relationships among basic index properties and the deformational response of sand.

These new developments will benefit several applications and geotechnical engineering problems. Some of the most urgent to address includes:

- *Tailings dams:* Tailings dams rank among the largest, and perhaps the most dangerous, engineered structures on earth. Past failures have caused human, economic and environmental tragedies of unacceptable dimensions. VR-testing will enable more reliable testing and improved definition of parameters for the tailings material, reduce uncertainties in the material characterisation and assessment of liquefaction potential, and thereby reduce the risk of failure.
- *Offshore Wind Turbines:* The geotechnical design of foundations supporting offshore wind turbines is often driven by the estimation of the permanent rotation during

the OWT lifetime. This depends on the accumulated strains in the soil, which in sand very much depend on the initial fabric when the sand is loaded. An improved understanding of the link between fabric and accumulated strains will enable a better estimation of the latter, thereby improving the design reliability, reducing the need to conservative design, and thereby reduce costs and increase safety.

4 SUMMARY AND CONCLUSIONS

The paper proposes a framework to develop Virtual Reality (VR) testing to supplement today's standard laboratory testing and highlights the key benefits of VR testing in geotechnical engineering.

New computational tools provide a promising technology that has the potential to become the core of Virtual Reality (VR) testing of granular materials. VR-testing is emerging as a novel and efficient alternative that will not only overcome some of the limitations and uncertainties in standard laboratory testing of sands, but also revolutionise the state-of-the-art for characterising and modelling the behaviour of sand, and thus closing the gap between grain interaction and the modelling of sand as a continuum.

To develop VR-testing to a level where it can routinely substitute physical laboratory testing, a great deal of innovative experimental, numerical and analytical research remains to be done, but the effort is well worth it, given the huge benefits that are expected for geotechnical design and practice from the development of VR technology.

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