Andrade, J. E. *et al.* (2012) ***Géotechnique Letters* 2**, 135–139, http://dx.doi.org/10.1680/geolett.12.00023

Multiscale 'tomography-to-simulation' framework for granular matter: the road ahead

J. E. ANDRADE*, I. VLAHINIĆ*, K.-W. LIM* and A. JERVES*

A roadmap is presented to transition seamlessly from an image to a predictive computational model for granular materials. So far, constitutive modelling in granular materials has been based on macroscopic experimental observations. Here, the point of departure is the basic granular scale where kinematics, contact forces and fabric control the macroscopic mechanical behaviour of the material. New computational and analytical tools are presented that allow for more accurate measurement of kinematics and inference of contact forces, directly from imaging tools (e.g. high-energy tomography). These grain-scale data are then used to construct powerful multiscale models that can predict the emergent behaviour of granular materials, without resorting to phenomenology, but can rather directly unravel the micro-mechanical origin of macroscopic behaviour. The aim of these tools is to furnish a 'tomography-to-simulation' framework, where experimental techniques, imaging procedures, and computational models are seamlessly integrated. These integrated techniques will help define a new physics-based approach for modelling and characterisation of granular soils in the near future.

KEYWORDS: constitutive relations; deformation; numerical modelling; plasticity

INTRODUCTION

Figure 1 shows the current modelling and characterisation paradigms at the grain scale and at the continuum scale. While significant progress has been made using continuum and discrete paradigms, much remains to be done. Specifically, one fundamental question remains: what is the micro-mechanical origin of macro-mechanical phenomena? It is argued that only a multiscale approach will be able to make the link across scales and help answer this question.

For the last five decades, granular materials have been studied using continuum mechanics. This paradigm, rooted mainly in plasticity theory (Schofield & Wroth, 1968), gave rise to powerful constitutive models. While the paradigm has proven useful, it crucially hinges on macroscopic diagnostics and elemental testing. Paradoxically, the main strength of the paradigm is at once its main weakness. Calibration based on macroscopic observations makes continuum models relatively robust and easy to use in engineering practice. The downside is phenomenology, which not only impacts the predictive capabilities when the models are stretched outside of their intended realm, but also masks the underlying physical causes of material response.

To escape phenomenology, over the past three decades material characterisation began to evolve from the macro towards the grain scales. For a time, observations were limited to photoelasticity using birefringent materials (Drescher & de Josselin de Jong, 1972; Majmudar & Behringer, 2005) and destructive techniques for natural geomaterials (Oda *et al.*, 2004). Within the last decade, however, the birth of in situ characterisation techniques (Desrues *et al.*, 1996; Alshibli *et al.*, 2003; Rechenmacher, 2006) has started to make it possible to extract particle kinematics (displacements and rotations) from X-ray computed tomography (CT) (Hall *et al.*, 2010), and inter-particle contact forces, by way of X-ray diffraction (Hall *et al.*, 2011). There is, however, much work ahead. Arriving at the full-field grain scale kinematics and forces requires the aid of a suite of computational tools, many of which are active topics of research today, as evident from Fig. 1.

The modelling paradigm has also gravitated towards the grain scale. Discrete element methods (DEM) have led the way, but have struggled to make a leap from the qualitative toward the quantitative. Accounting for particle shape appears to be an important ingredient and DEM has seen significant work in this area in the last three decades (e.g. O'Sullivan (2011) and references therein). Primarily, there is a lack of concerted validation efforts to compare results from DEM simulations, at the micro and macro levels, against experiments on natural materials, such as sands.

Translating the experimental and computational gains made at the grain scale into the macroscopic realm is another challenging topic. As shown in Fig. 1, grain scale kinematics and forces must somehow link to macroscopic stresses and strains by way of multiscale methods. In this regard, the central question is the following: which details are important and what information should travel between the scales. It is clear that millions of degrees of freedom (grain kinematics and forces) emanate from an assembly of grains. How does one reduce this to a six-dimensional space of stresses and strains over a unit cell? The following sections present a roadmap of a concerted and integrated effort towards this goal. It should also be noted that, at least for the time being, the proposed approach is limited to coarse-grained cohesionless materials (e.g. sands).

MULTISCALE 'TOMOGRAPHY-TO-SIMULATION' FRAMEWORK: A VISION

In granular materials, micro and macro descriptions of mechanical state are intimately coupled. However, as

Manuscript received 4 May 2012; first decision 5 June 2012; accepted 12 July 2012.
Published online at www.geotechniqueletters.com on 28 September 2012.
*Applied Mechanics, California Institute of Technology, California, USA

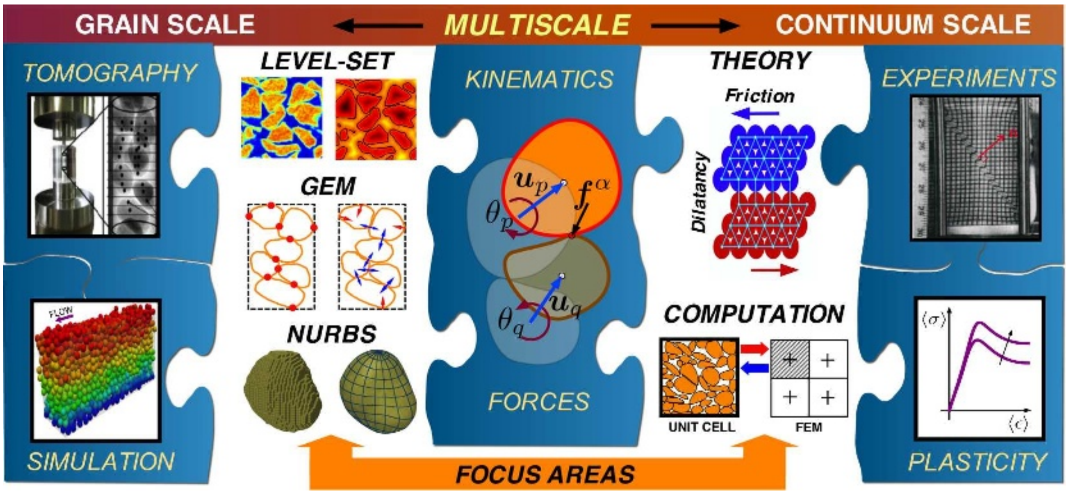

Fig. 1. Schematic showing unified tomography-to-simulation framework across scales (left to right) and integration of characterisation and simulation (top to bottom). Areas of relatively established understanding (shown in solid puzzle pieces), such as grain-scale tomography and simulation, are contrasted with focus areas that need major developments. Level sets, GEM and NURBS are key computational ingredients to enable grain-scale characterisation and simulations, which yield particle kinematics and forces. Using such quantities, multiscale methods provide the link between experiments and continuum plasticity models to complete the proposed framework. Multiscale methods hinge on theory and computations to extract central physical parameters such as friction and dilatancy using data obtained by characterisation and simulation at the grain scale. Kinematics here are represented by the particle translations u_p and u_q and angular rotations θ_p and θ_q for two particles p and q that share a contact point with corresponding force f^α. Portions after Alshibli *et al.*, 2003; Andrade & Tu, 2009; Andrade *et al.*, 2012a; Hall *et al.*, 2011

shown in Fig. 1, the modelling and characterisation remain compartmentalised, as exemplified by a relative lack of connection between experiments and modelling at the grain scale, as well as across scales. For instance, DEM has interacted very little with continuum approaches based on plasticity.

The present paper proposes a vision for a multiscale 'tomography-to-simulation' framework where artificial boundaries between characterisation and modelling campaigns across scales are diluted. As shown in Fig. 1, it is advocated that the way to prediction is a complete amalgamation between characterisation and simulation across scales and present 'focus areas', where major developments are needed in order to complete the puzzle. Also shown in Fig. 1 are areas where historical strength is currently present (e.g. plasticity) and areas where strength is increasing rapidly (e.g. tomography). It is argued that the way forward is the development of new methods that can furnish the missing pieces, such that the characterisation and simulation of mechanical state at the grain scale can be *validated and quantified,* and subsequently *linked* to the description of mechanical state at the continuum scale. This is very much work in progress and includes the study of the 'meso' or intermediate scale, whereby interactions between *groups* of grains may contribute to the overall constitutive picture (e.g. Tordesillas *et al.*, 2011).

The following sections showcase embryonic attempts to furnish some of the missing pieces of a unified 'tomography-to-simulation' framework. The point of departure is the grain scale and its characterisation and simulation. Tomography and DEM are used as prototypes for grain scale characterisation and simulation, respectively. At the continuum scale, macroscopic experimentation and simulations based on plasticity are used as prototypes. A vision is presented for how the proposed framework could fully unravel grain scale mechanics, including kinematics and forces, and how these in turn could help inform continuum scale material response.

CHARACTERISATION OF KINEMATICS AND CONTACTS ENABLED BY COMPUTATIONS

Successful inference of kinematics and contacts has several crucial applications:

(*a*) unravelling of grain kinematics and grain fabric, including contact evolution during loading, integral to the evolution of strength in granular systems as shown in the multiscale section
(*b*) inference of contacts locations provides a necessary and important input for a technique that could deliver contact forces in opaque granular systems by way of X-ray diffraction (Hall *et al.*, 2011; Andrade & Avila, 2012)
(*c*) inference of grain shapes that are representative of true particles shape (to sub-image resolution) provides a natural stepping-stone toward a new generation of DEM that can account for arbitrary particle shape, as described in the next section (Andrade *et al.*, 2012b).

The present paper showcases a tool to help in the characterisation of kinematics and contact.

Figure 2 shows an example of a triaxial compression test using in situ three-dimensional (3D) X-ray computed tomography (3DXRCT). Besides stress and strain data acquired during direct macroscopic testing, 3DXRCT provides images of microstructure at distinct load stations. Sophisticated techniques are needed to make the data palatable for mechanical analysis; that is, to translate image voxels into grain fabric and morphology. Watershed technique has been a trusted workhorse in these applications (Soille, 2003). The technique ultimately furnishes grains that are segmented from the voids, and from each other.

Watershed, however, has a subtle but damaging drawback – it is required to operate on and output binary images, a penalty of a successful segmentation. This is problematic for two reasons. The first is that binary images introduce artificial roughness to grain surfaces, complicating a direct tomography-to-simulation paradigm (DEM prefers smooth particles for contact detection) and often

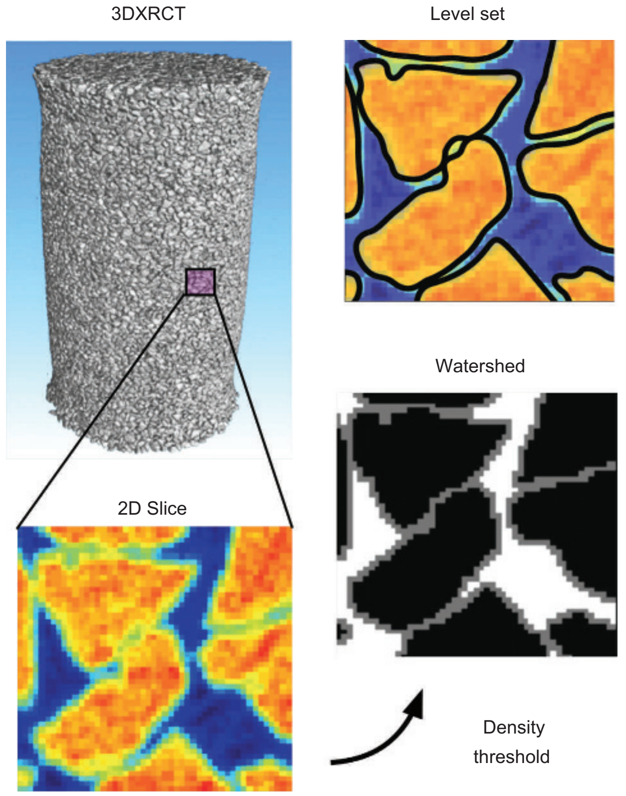

Fig. 2. Methods for inferring accurate grain shape and fabric from experimental data. (Left) An example of a 3D X-ray image containing thousands of individual grains (after Hall *et al.*, 2010) with a full-fidelity 2D slice shown below. (Right lower) Segmented 2D slice of a full 3D image showing the shortcoming of the current segmentation techniques. Grain boundaries are stepped (binary) and resolution of the contact regions is highly degraded after thresholding (grains appear fused). (Right upper) Grain boundaries detected using levelset technique (after Vlahinić *et al.* (2012)). Gradients of a full-fidelity image 'guide' the grain boundaries to their final location. Starting guess is provided by watershed

supplying inadequate resolution for inference of grain rotations (e.g. see Andó *et al.* (2012)). The second, and more critical drawback, is the removal of details about the location and orientation of inter-particle contact, as shown in Fig. 2. Our current inability to characterise this aspect of granular behaviour significantly impedes our understanding of the physical sources of strength (as opposed to kinematics or strains only).

The first strides toward overcoming the aforementioned drawbacks of watershed have been made recently (Vlahinić *et al.* (2012)). The proposed methodology uses active level sets directly on high-fidelity tomographic images to delineate grain surfaces and contact locations. In this way, the final grain boundaries are smooth and representative of true grain shapes to sub-voxel resolution, and without 'melted' (oversegmented) contact regions, as shown in the lower right portion of Fig. 2.

GRANULAR ELEMENT METHOD (GEM): COMPUTING GRANULAR KINEMATICS AND CONTACTS

Besides characterisation, there is a need for *quantitative* simulation of kinematics and contact forces in real granular materials. Existing DEM approaches account for particle shape by way of clustering (e.g. Matsushima *et al.,* 2009), polyhedra, potential particles, superquadrics (O'Sullivan, 2011). While these approaches have improved the shape representation capabilities of DEM over discs and spheres (Cundall & Strack, 1979), computational results today remain mostly qualitative. DEM's predictive capability will directly depend on its ability to capture real particle morphology. At the same time, the connection of particle morphology with macroscopic properties of geomaterials, for example permeability and strength, is well established (Cho *et al.*, 2006; Garcia *et al.*, 2009).

We have recently taken steps to use non-uniform rational basis splines (NURBS) (Piegl & Tiller, 1997) for representing grain shapes in computational models. In this way, the resulting DEM model, termed granular element method (GEM), can directly account for arbitrary particle shapes and vary features such as sphericity and roundness (Andrade *et al.,* 2012b). This key idea is illustrated in Fig. 3.

GEM also provides a direct bridge between experimental tomography (e.g. 3DXRCT) and DEM computations. Representative grain morphology obtained using the segmentation process described previously, can be used as a direct input into GEM. As such, GEM bypasses complicated and ad-hoc approaches needed to approximate true particle shape (e.g. clustering) and performs direct computations on natural grain shapes.

In the two-dimensional (2D) implementation of GEM (Andrade *et al.*, 2012b), grain shapes are described by NURBS of cubic degree and shape flexibility is achieved

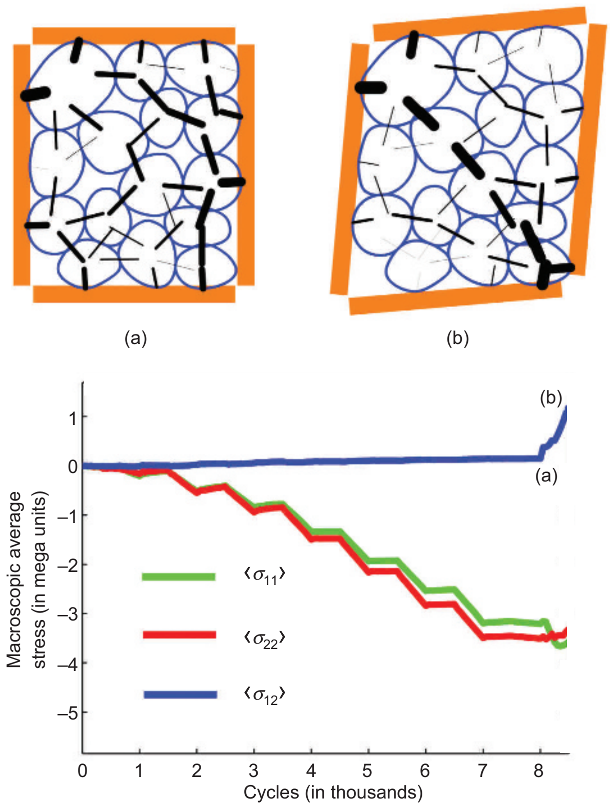

Fig. 3. Grain scale simulation of isotropic compression (a) followed by constant-volume shear deformation (b) using granular element method (GEM). Surrounding walls are rigid and frictional. Solid lines are interparticle force vectors. Bottom plot shows evolution of stress components. It can be seen that the macroscopic stress remains hydrostatic until the end of the isotropic compression with the two normal components fairly close to each other and the shear component close to zero. Constant-volume shear deformation subsequently induces an increase in shear stress, with the normal stresses fluctuating slightly. After Andrade *et al.* (2012b)

using control points, knots and weights. Contact algorithm and update of grain kinematics are performed directly on NURBS. A numerical example of the method is shown in Fig. 3, where a 2D assembly of arbitrary shaped particles is subjected to uniform compression followed by shear deformation. The example illustrates the ability of GEM to obtain kinematics and contact topologies that are reflective of the real granular assemblies.

Extension of GEM to 3D using particle morphologies inferred from 3DXRCT data is currently underway. The current authors are motivated by the possibility of performing simulations that are comparable in fidelity with 3DXRCT-based experiments.

GRANULAR-SCALE ENHANCEMENTS TO CONTINUUM: MULTISCALE ANALYSIS

Once particle kinematics and forces are inferred experimentally or by simulation, as shown above, the main challenge is the transmission of this information to higher scales. What is the fundamental set of information to be passed between scales in a discrete-continuum material? From the macro to the micro, one can imagine passing the state (stress, strain, history), but from the micro to the macro, this question is not trivial and will determine the success of the multiscale approach. One approach is to exploit the micro-mechanical state to extract physical macroscopic parameters. For example, friction and dilatancy have recently been proposed as two potentially crucial parameters that can be extracted directly from the micro-mechanical information (Andrade & Tu, 2009). Figure 4 shows a schematic of the hierarchical scheme that can be utilised to link the grain and continuum scales. At the continuum level, one can use basic models such as Mohr–Coulomb that depend on fundamental parameters such as friction and dilatancy and that can be extracted directly from the micro-structure.

Efforts are currently underway to obtain more realistic

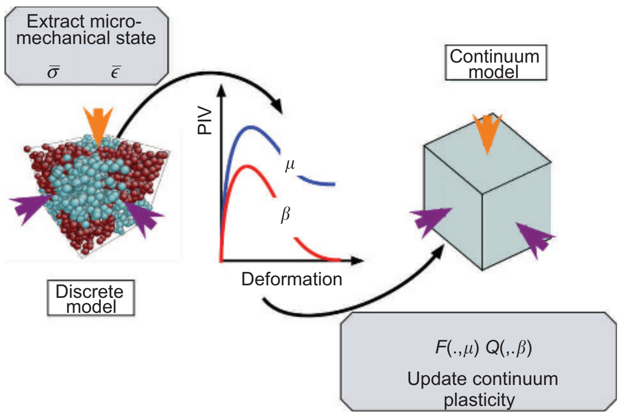

Fig. 4. Schematic of hierarchical multiscale procedure. At the grain scale there is a discrete system furnished by a model (e.g. GEM) or an experiment (e.g. 3DXRCT). At the continuum scale there is a plasticity model (e.g. Mohr–Coulomb) engrained into a finite-element framework. Multiscale extracts plastic internal variables (PIVs) such as friction μ and dilatancy $\beta$and infuses their evolution into the continuum plasticity model using the yield surface F and plastic potential Q. In this way, multiscale models bypass phenomenological hardening laws typically employed in plasticity and instead update the evolution of macroscopic plasticity based on grain scale physics. For example, using this approach particle kinematics from 3DXRCT have been used directly to calculate dilatancy in plasticity models to simulate successfully macroscopic experimental results in Andrade *et al.* (2011)

models based on a multiscale philosophy, for example Dascalu & Cambou (2008), Wellmann *et al.* (2007), Nitka *et al.* (2009). Even though researchers have been looking for the connection between micro and macro behaviour, for example Oda & Iwashita (1999) and references therein, real progress did not take place until the last decade or so. Two major factors have contributed to this paradigm shift: increased computational power and advanced visualisation (e.g. 3DXRCT). As elucidated in the previous sections, once kinematics and inter-particle forces are obtained using either experiments or computations, this information can potentially be used to formulate or inform continuum models.

The linkage between grain and continuum scales can be furnished by average measures that are well established (see Oda & Iwashita, 1999). For instance, the average stress in an assembly of particles is given by Christoffersen *et al.*, (1981)

$$\langle\sigma\rangle = \frac{1}{V}\sum_{\alpha=1}^{N_c} f^\alpha \otimes d^\alpha$$

where V is the total volume of the unit cell assembly containing N_c contact points, f^α is the contact force at the αth contact point and d^α is the branch vector connecting the centroids of the two particles in contact at the α point. This expression furnishes a bridge between a continuum quantity, such as the stress tensor $\langle\sigma\rangle$, and grain scale interparticle contact forces f^α and the influence of fabric implied by d^α. A similar expression is available for average strains $\langle\varepsilon\rangle$ (Bagi, 1996) and is linked to the grain-scale kinematics. Recently, Andrade *et al.* (2011) have used these bridges to extract friction and dilatancy *directly* from DEM simulations and advanced experiments using 3DXRCT. In this way, phenomenological hardening laws are bypassed and physical (macro) parameter evolutions are obtained directly from grain-scale mechanics.

As shown in Fig. 1, the development of multiscale techniques hinges on the calculation or measurement of grain kinematics and forces. This requires accurate discrete element models, such as GEM, and advanced characterisation techniques that can accurately infer kinematics and forces. As shown above, the linkage with computational techniques is crucial for tomographic characterisation methods to yield *quantitative* kinematics and forces that can then be *linked* to the continuum scale using multiscale techniques. These areas are central for a unified framework and are in need of significant development.

CONCLUSIONS

The present paper presented a vision for a unified 'tomography-to-simulation' framework for characterisation and modelling of granular materials across scales. The proposed approach advocates for erasing the artificial boundaries traditionally erected when modelling and characterising granular soils. With a unified methodology that can connect grain and continuum scales and utilise characterisation and modelling synergistically, it will be possible to develop predictive tools in the near future. There are several focus areas where work is needed to achieve this goal, but the road ahead looks promising.

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