A Report on Research Trends in Mechanics:

"REPORT ON RECENT TRENDS IN GRANULAR MECHANICS"

US National Committee on Theoretical and Applied Mechanics (USNC/TAM)

Granular Materials Committee, Engineering Mechanics Institute
Mustafa Alsaleh[1], Ching S. Chang[2], Ali Daouadji[3], Usama El Shamy[4], Mahdia Hattab[3],
Pierre-Yves Hicher[5], Matthew R. Kuhn[6], Shunying Ji[7], Bo Li[8], Shuiqing Li[9], Anil Misra[10],
Jean-Noel Roux[11], Antoinette Tordesillas[12], Xu Yang[13], Zhen-Yu Yin[14], Zhanping You[15],
Mourad Zeghal[16], Jidong Zhao[17]

OVERVIEW

Granular materials are complex systems that are receiving intense interest within the engineering, physics, and mathematics communities. These ubiquitous materials play a significant role in geosystems, mining, petroleum storage and extraction, ceramics engineering, and pharmaceutical science. The report reviews recent developments and new advances in experimental, computational, and modeling methods that extend understanding to a wide range of materials and phenomena: multi-phase systems with strong solid-fluid interactions; multi-field systems in which van der Waals and electrical fields gain dominance; and bonded granular systems for advanced pavements. Experimental advances include computed neutron and nanometer scale tomography, magnetic resonance imaging, refractive index matching, digital image correlation, and acoustic emission analysis. Complex systems and data mining tools are now being used to extracting meaningful information and patterns from data. The state of the art in continuum modeling has shifted to micromechanical or multi-scale approaches with developments being made from three perspectives: constitutive modeling enhanced by material fabric and fabric evolution; modeling discrete systems as equivalent continua; and computational multi-scale modeling. Advances in computational modeling and parallel computing are exploited to model the complexities of grains and contacts, and to study strongly coupled grain-fluid systems using computational fluid dynamics and particle-structure interactions using combined discrete and finite element methods. This report focuses on three broad advances in granular mechanics: the experimental imaging of granular materials (Part I); the transition between micro-, meso-, and continuum-scale modeling (Part II); and the modeling of multi-phase materials (Part III).

---

[1] Caterpillar Inc., Mossville, IL, USA
[2] Dept. of Civil and Env. Engrg., Univ. of Massachusetts, Amherst, MA, USA
[3] Lab. de d'Etude des Microstructures et de Mécanique des Matériaux, Université de Lorraine, Metz, France
[4] Dept. of Civil and Env. Engrg., Southern Methodist Univ., Dallas, TX, USA
[5] Res. Inst. in Civil and Mechanical Engineering, Ecole Centrale de Nantes, France
[6] Dept. of Civil Engrg., Shiley School of Engineering, Univ. of Portland, Portland, OR, USA
[7] Dept. of Engrg. Mechanics, Dalian Univ. of Tech., China
[8] Dept. of Civil and Env. Engrg.. Rensselaer Polytechnic Inst., Troy, NY, USA
[9] Dept. of Thermal Engrg., Tsinghua Univ., China
[10] Dept. of Civil, Env., and Arch. Engrg., Univ. of Kansas, Lawrence, KS, USA
[11] Université Paris-Est, Institut Navier, Champs sur Marne, France
[12] Dept. of Mathematics and Statistics, Univ. of Melbourne, Australia
[13] Dept. of Civil and Env. Engrg., Michigan Tech. Univ., Houghton, MI, USA
[14] Ecole Centrale de Nantes, France
[15] Dept. of Civil and Env. Engrg., Michigan Tech. Univ., Houghton, MI, USA
[16] Dept. of Civil and Env. Engrg.. Rensselaer Polytechnic Inst., Troy, NY, USA
[17] Dept. of Civil and Env. Engrg., Hong Kong Univ. of Sci. and Tech., Hong Kong

Part I. Experimental Advances in Micro-scale Imaging

For decades, engineers have designed industrial processes, building foundations, and structures by using specimens of a scale much smaller than the full prototype size. A new paradigm is achieved where materials can be tailored for different needs in engineering practices. The methodology to reach this goal is through a dialogue between modeling and experimentation. With granular materials, the microstructure, however complex, is now being examined, modeled, and simulated with greater fidelity to its true composition and behavior. The complex microstructures of these highly heterogeneous materials are now being investigated and understood at multiple scales. New experimental facilities allow *in situ* and post-mortem analyses with a very high resolution to reveal the complete 3D structure.

By using destructive techniques such as scanning electron microscopy (SEM) and transmission electron microscopy (TEM), granular micro-structures can be imaged at microscopic and nanoscopic scales. SEM techniques need completely lyophilized samples to study the stress-dependent microstructure and its evolution (Fig. 1) by quantifying the orientation of clay particles [1-3]. For example, TEM observations are now used to quantify deformability at the scales of particles and particle layers with high precision to identify effects related to creep phenomena. Recent developments in measurement techniques and the high resolution of images also allow visualization of even nano-scale structures as was not previously attempted. This imaging of the grains has been augmented by recent work by Delage [4] and others, who have used mercury porosimetry tests to provide a precise characterization of the microstructural pore network and its changes during mechanical loading.

Non-destructive methods also permit non-invasive analyses during loading. Using the Acoustic Emission (AE) technique, it is possible to localize kinematic discontinuities such as cracks in bonded materials [5] or grain breakage in discrete materials and to follow their evolution. Most acoustic emissions are damage-related, and the monitoring of each emission is used to predict material failure. However, this technique is not able to precisely predict the position of the crack or breakage, as AE only detects activity inside the specimen. To complement this method, ultrasonic wave propagation precisely follows the evolution of elastic properties at the level of micro-strains and smaller. Progress has also been made in calibration and in analyzing the data obtained during testing [7]. Most of these studies have used devices equipped with acoustic transducers in contact with the material so that compression waves and shear waves can be recorded during the mechanical loading.

One of the most promising techniques is micro computed tomography (micro-CT), enabling the visualization of the microstructure with a high precision. X-Ray micro-CT is able to capture the morphology of the grains and, using relevant tools for thresholding and segmentation, even locate and define the contacts between grains [7]. Displacement and rotation of individual grains and therefore fabric evolution are experimentally established. The penetration of fluids (e.g. water or pollutants) inside porous materials is an important development when dealing with transport or depollution research. X-ray micro CT is limited, however, because the fluid of interest and porous medium through which the fluid is moving may have similar levels of X-ray attenuation, which limits the image contrast. Magnetic resonance imaging (MRI) is an optional technique that has recently been exploited. This technique, however, cannot always be used to establish absolute values for the moisture content within a system, in particular at low saturation contents [8]. High-speed neutron tomography has been recently introduced as a visualization technique for fluids inside porous materials, which can be used as a complementary technique to X-ray tomography since elements such as hydrogen, having a weak attenuation for X-rays, are detected with neutrons. Volumes of the scanned specimen can be meshed and exported to finite element software. Such volumes can be considered as representative volume elements (RVEs) within the context of two-scale finite element (FE2) methods, avoiding the use of postulated constitutive relations for solving boundary value problems (see part II).

Digital Image Correlation (DIC), as another images-based technique, is a full-field image analysis method, which is based on grey-scale analysis of digital images. It allows determining the displacements of an object subjected to mechanical, thermal or hydraulic load in three dimensions. Although limited to observations of granular specimens along an exposed surface, DIC gives a precise picture of the disordered and collective behavior at the local scale (i.e., grain scale for granular media and particle/agglomerate scale for clayey materials) under small and large deformations (<100%) for triaxial and biaxial apparatus [9].

Part II. The Micro-meso-macro Transition

Recent advances in characterizing particle-scale images have enabled an improved understanding of the relation between micro-scale and bulk behaviors. Unlike simplistic early analyses which assumed that grains were rigid and that entire sheets of grains would uniformly slide across adjacent sheets, modern analyses recognize the highly heterogeneous nature of deformation and stress transmission, characteristics that have been revealed in high resolution imaging (as in the previous section) and in computer simulations (as described below). Grain movements are highly coordinated, and the movement of any single particle is influenced by a surrounding zone of several dozens or hundreds of particles. Recognition of the mechanics within this meso-domain is key to resolving the micro-macro relationship, and for ultimately developing reliable constitutive relations. This understanding will also enable the design of granular materials to serve a range of requirements by manipulating grain-scale characteristics and the arrangements of particles.

Rheological regimes

In modeling the transition from micro to macro, it is essential to consider the rheological flow regime to which the model applies. Early works essentially recognized only two regimes: slow quasi-static deformation and rapid collisional flow. We now recognize a range of behavior that transitions between these two extremes.

Understanding the rheophysics of granular materials, i.e., their macroscopic mechanical properties in relation to the microscopic mechanisms of deformation and flow, is still a major challenge. Dense states, in particular, exhibit particularly strongly disordered properties in the force field patterns (i.e., the "force chains" that have been observed for several decades [10]) as well as in the displacement or local strain fields (which exhibit long-ranged correlations [11,12]. This heterogeneity makes it especially difficult to relate macroscopic properties to microscopic ones. Microscopic approaches to granular mechanics have recently benefited from discrete, grain-level numerical simulations (DEM), which can reproduce the essential rheological features of granular materials [13] with simplified grain geometries and interaction laws. Yet such approaches introduce many parameters, the number of which further increases as models of growing sophistication, involving adhesion [14], rolling resistance [15,16], or various particle shapes [17,18] are considered.

Dimensionless measures: Typical rheological tests involve a confining stress, say a pressure P, some strain rate ε imposed onto an assembly of grains with mass m and diameter d. Contact interactions are most often described with at least two stiffness parameters (for normal and tangential forces), in addition to friction and, possibly, rolling friction [16], as well as viscous terms opposing the relative motion of contacting grains. Adhesion [14] introduces two additional parameters, a force scale F_0 and an attractive range D_0. All of these quantities are conveniently combined into suitable dimensionless groups, which might then be used to delineate different rheological ranges and express constitutive relations in a convenient form.

While assembling processes such as pluviation, depend in a complex way on many microscopic features of the mechanical model, quasistatic deformation and dense, inertial flows of granular materials are primarily controlled by grain shape and by friction (including, possibly, rolling friction), to which two dimensionless numbers should be added. The inertial number I, combining strain rate, confining stress, and particle mass, quantifies inertial effects and defines the approach of the slow, quasistatic limit (the limit of vanishing I). The stiffness number, κ, compares confining forces and contact stiffness, thereby expressing the typical contact elastic deflection relative to grain diameter, proportional to $1/\kappa$. The rigid grain limit, in which elastic properties become irrelevant, is that of infinite κ.

For cohesive grains, a third dimensionless group, a reduced pressure $P^*=Pd^2/F_0$, expressing the relative importance of confining stress and contact adhesion, should also be introduced. For small P^*, depending on their assembling history, granular assemblies, in which adhesion dominates over confining forces, might equilibrate at very small solid fractions, with a fractal structure at small scale, similar to colloidal aggregates [14]. Under growing external stress and P^*, the collapse of tenuously connected, loose structures, results in plastic irreversible compaction, until the density and the morphology of cohesionless systems are retrieved under large enough P^*.

In DEM simulations of cohesionless systems, the level of plasticity in isotropic or oedometric compression of sands observed in the laboratory is only obtained with breakable grains, for which grain strength is an essential additional characteristic. In view of its importance for soil mechanics, grain breakage modeling is an active field of research ([19], also described below).

Two rheological flow regimes: Even in cohesionless systems, for which microstructure has been more thoroughly explored, the correspondence between microscopic and macroscopic mechanical properties reveals surprises, as many aspects of the material rheology are more sensitive to the geometry of the grain packing than to contact mechanics. In particular, we must avoid the naïve analogy between the gradual, elasto-plastic mobilization of internal friction at the macroscopic scale and the mobilization of contact friction at the microscopic scale – as is certainly apparent in the extreme case of frictionless grains, which have internal friction, but no dilatancy [20]. The dependence of basic macroscopic properties such as internal friction and dilatancy upon the inter-granular friction coefficient are now rather well-known (as briefly recalled in [21]) but still incompletely analyzed and explained. Such properties are most often discussed in the critical state, i.e. in a steady state with monotonically growing quasistatic deviatoric strain. The lack of sensitivity of granular mechanics in solid-like materials or dense flows to many parameters of contact interactions, such as viscous dissipation (or coefficients of restitution) and details of tangential elasticity is a favorable situation for modeling. The critical state, in particular, is only dependent, provided the contact stiffness is reasonably large and the particles are durable, upon grain shape, size distribution, and the contact friction coefficient.

Successful rheological models of dense granular flows have emerged in the past decade [22] based on the description of steady shear flows as generalized, I-dependent critical states, with an I-dependent internal friction coefficient and solid fraction tending to their static values as I decreases to zero. Several research groups (see e.g. [23]) are implementing the resulting laws in continuum fluid mechanics computations of dense granular flow in various geometries. As opposed to the critical state, or its analogs in the presence of inertial or viscous effects, the assembling process, from a fluidized initial configuration, of an equilibrated, pre-stressed granular pack, is sensitive to many micromechanical details (including coefficients of restitution) and results in history-dependent structures, varying in density, inherent fabric anisotropy, and also, independently from the density, in coordination number [24].

Two regimes of slow loading: The response of equally dense systems to increasing deviatoric loads in slow quasistatic conditions highlights the important distinction between two different rheological regimes [25,26]. In the first regime (regime I), which might extend from zero strain to a large fraction of the maximum deviator stress, macroscopic strain is due to micro-scale material strain in the contact regions of the grains and in contact deformations. The macroscopic (elastoplastic) stiffness of the material scales with the (elastic) contact stiffness. Thus, models assuming perfectly rigid grains, as in the Contact Dynamics (CD) simulation method [26], predict a rigid macroscopic response, with no strain at all. Regime I ends as soon as the initial contact structure breaks, and the subsequent strains result from repeated micro-instabilities within the system, which continuously produces relaxations and repairs during the loading process. Macroscopic deformation is determined by packing geometry and is insensitive to contact stiffness. The occurrence of these two rheological regimes, the first one being confined to small strains and stiff responses observed upon changing the load direction, but possibly extending to significant stress intervals, should be explored in order to better understand the relations between fabric evolution and strain. Micro-instabilities in the second regime (regime II) have not yet been fully studied [27,28], but the mechanisms by which they rearrange contact networks contain essential information at the micro scale. The distinction of those two regimes should also provide useful indications in investigations of instabilities leading to strain localization or collapse.

Primary dimensionless numbers – most notably I, κ, and P^* – are essential in distinguishing those rheological regimes that must still be explored (for example, loose cohesive systems in response to deviatoric loads) or require a more complete understanding (the quasistatic regime II). Finally, the dimensionless characteristics described above apply to the regime of dense flow; whereas, flow in the diffuse collisional regime is differentiated by the mean free path of particle collisions, as characterized by the Knudsen number [156].

Unraveling granular complexity from data

As in many complex systems in nature, society, or technology, rapid advances in experiments and simulations of granular rheology are changing the way we gain knowledge from data. In the field of granular media mechanics and physics, developments in the mathematics and statistics of complex systems, underpinning many of the techniques in data mining, have recently gained traction. Arguably the prime catalysts for this change are the increasingly large and complex data sets from high-resolution measurements and simulations [7,10-13,29-31]. As discussed in Part I, the past decade has witnessed transformative progress in the imaging of a deforming granular material down to the scale of individual grains and associated pores, from which various properties (e.g., contacts, kinematics, contact forces) can be measured over many and finer time steps of a loading history. Resultant data sets have steadily increased in volume and dimensionality. Effective use of these assets rests on new perspectives, tools and ideas in data analysis – beyond traditional statistical methods. In particular, new methods are needed to extract useful patterns across many length scales in space and time, as well as quantify uncertainty and test for the robustness of patterns, given the imperfections ("artifacts") of real world data. Recent trends have demonstrated the efficacy of various amalgams of complex systems (CS) techniques in achieving these research needs for a broad range of data for dense granular systems, from simulations to experiments on synthetic and natural granular materials.

The approach often begins with representing the deforming material as an evolving graph or complex network [32-38]. Here the multidimensional data (with time as one of the dimensions) is mapped to a graph comprising nodes (e.g., grains, pores or clusters of these basic units) and links (e.g., physical contacts between grains [33-36], pore throats, or similarities in properties [37,38]). This abstract, topological representation of the material enables the use of complex networks (CN) to extract useful knowledge across spatial scales. In these studies, CN is often employed together with other complex systems techniques such as dynamical systems (DS), information theory (IT), and network flows (NF) to uncover details across temporal scales (e.g., phase transitions) as well as evolution rules in the observed spatial patterns. The tools of combinatorial optimization (CO) and structural mechanics (SM) provide an avenue to identify the interconnections between structural stability, topology and dynamics, in turn, giving insights into mechanical function [39,40].

Characterization of fabric and force evolution using complex networks: The most frequently studied network in granular systems is the contact network. Here, the grains are the nodes and the contacts are the links. Fabric anisotropy and its evolution manifest in the changing topology of this network. Topology can be summarized succinctly through various complex network measures (e.g. degree, path length, clustering coefficient) [33-36,39-42]. Information on force anisotropy can be introduced by weighting each link by a physical quantity (e.g., contact force, strain energy). The coupled evolution of fabric and force anisotropy can then be probed using generalized network measures (e.g. strength, sub-graph intensity). These network measures have revealed insights into how, in response to applied loads, dense granular materials regulate their contacts and "select" which of these transmit strong versus weak forces.

Deformation as a process of self-organization: A defining aspect of complex systems is their propensity for self-organization, and granular materials are no exception. A study of the recurring patterns in the contact network ("motifs") has uncovered the structural building blocks of self-organization in systems undergoing localized versus diffuse failure [41-43]. One outcome has been the quantitative characterization of cyclic building blocks (i.e., the minimal cycles) and their synergetic co-evolution with linear building blocks, the primary load-bearing force chains. Arevalo et al. [29] showed that 3-cycles are the mechanical structures that give rigidity to granular systems. Viewed from structural mechanics, the material essentially self-organizes to form a lattice of "truss-laced columns" with high compressive load-bearing capacity. Triangular trusses brace the force chain columns, both to increase rigidity and stability where needed (i.e. prop-up column misalignments) and to resist relative grain rotations (i.e., the precursory mechanism for force chain failure by buckling) [41]. When viewed at the scale of a grain and its first ring of neighbors, this complex interplay between forces and contact topology is reminiscent of "magic-number behavior" observed in molecular self-assembly [40,42]. To support axial loads, force chains typically reside in more stable states of the stability landscape, preferring stabilizing truss-like, three-cycle contact triangular topologies with neighboring grains. The most likely conformational transitions during force chain failure by buckling correspond to rearrangements among, or loss of, contacts that break the three-cycle topology [42]. This pattern of cooperative evolution between force chains and 3-cycles proved robust at multiple length scales for different materials, loading conditions, dimensionality and mode of failure [40-43]. Indeed, the remarkable similarities in the evolution of function and the prevalence and persistence of minimal cycles and force chains in these systems suggest that these structures and their co-evolution form a generic feature of dense granular systems under quasi-static loading.

New insights into granular phase transitions using dynamical systems: Spatio-temporal patterns in force transmission [30,44] and contact "network motifs" (recurring patterns in networks) [45] have proved pivotal in the transitional regimes of the granular "phase diagram" [46-47]. Shear-jamming, reminiscent of shear thickening in fluids, was recently found in the quasi-static limit of this phase diagram [30]. Using photoelastic disk assemblies, it was discovered that shear forces –

which usually break-up materials and induce failure – could drive a granular material to become solid-like or “jam” at a fixed density. Shear-jamming exhibits a rich phenomenology. For small applied shear stresses, the states are “fragile”. A minimum shear stress is needed to achieve robust, shear-jammed states in which the strong force network percolates in all directions. While the related concepts of “rigidity”[33], “jamming”[30] and a “percolating force network” [10-12,30,44] have attracted significant recent attention in the physics communities, these have also been observed in soil and rock and studied as “percolation phenomena” in the geomechanics and geophysics communities [48,49]. In recent experiments on compaction, consolidation and triaxial shear, sand-clay mixtures presented a similar percolation behavior, yielding clues to the role that each soil fraction plays in transferring forces through the medium [48]. As the fraction of the stiffer sand particles is increased, an abrupt transition was observed from clay-like to sand-like behavior over a relatively narrow range of sand (coarse) fractions (45-48%). At this transition, the clay (fines) fills the pores with limited effect on the mechanical response of the mixture. Force chains, as yet, cannot be observed directly in natural granular materials. Regardless, analysis of the sand in terms of its component void ratio where clay is considered as a part of the void space gives direct evidence that any load applied to the mixture is transmitted through chains of mainly sand particles (i.e. percolating force chain network). The fines provide the force chains providing the necessary lateral support to resist buckling.

In [46], dense granular systems from about 100 tests (including those on sand and photoelastic disk assemblies in [7,30-31,38]) were recently shown to exhibit preferred structural ordering of four-node subgraphs in the contact network reminiscent of a “superfamily” classification. This classification, robust against moderate levels of observational noise [50], can be used to map boundaries in a so-called jamming phase diagram [46], thus offering an opportunity to bridge the mechanics and physics perspectives on the constitutive behavior of granular systems: i.e., pre-failure versus failure regimes in soil mechanics or jammed versus unjammed regimes in physics.

Another dynamical systems technique, introduced to detect subtle changes in nervous system dynamics after acute brain trauma [51], was used to characterize force transmission patterns in a prolonged cyclic shear test [49]. Aging was observed, and shear-jamming proved to be the underlying mechanism. The shear drives the sample to frequent the shear-jammed regime and therein inhabit a truss-laced lattice structure in which columnar force chains are reinforced by triangular (3-cycle) and rectangular (4-cycle) truss-bracing. These and other measurements of contact forces in 2D and 3D, for hundreds to thousands of stages of a loading test suggest there is now opportunity to comprehensively explore the granular phase diagram and to manipulate granular behavior from the grain scale.

<u>Boundary size matters:</u> Studies of granular response to shallow penetration by a punch [52] and a buried grain intruder [53] uncovered previously unknown commonalities, as well as differences in the patterns of force transmission between these systems and fully confined standard soil mechanics tests (e.g., biaxial and triaxial compression). Commonalities include: a) force chains are always better supported with contacts rich in 3,4-cycles than non-force chains; b) long force chains of six or more particles carry higher loads; and c) stable persistent 3-cycles preferentially degrade in the region where the shear band ultimately develops, leading to their complete depletion in the band at the onset of the critical state regime. Differences include: a) long force chains are buttressed against solid boundaries and clustered in space, consistent with recent observations in cone penetration tests [64], while short force chains are more uniformly spread, executing load transfer paths; and b) dilatancy is confined to distinct sub-regions of the shear zone. When a solid intruder is reduced to the size of a grain, structural evolution strongly correlates with failure: e.g., sharp drops in 3-cycle population coincide with bursts in kinetic

energy and the concomitant drops in resistance to the moving intruder [53]. Also, undeforming "dead zones", common in soil penetration tests, cease to exist, and the range of influence of the grain intruder converges to around 8-10 particle diameters, consistent with recent findings on the length scale of information (i.e. rotation) propagation in a dense sample [55].

New insights on initiation and propagation of failure: Successes in geomechanics on measuring contacts and grain kinematics using X-ray microtomography [7] have led to new insights into failure evolution. The complex network metric of closeness centrality (CC) was used to extract the hidden patterns from data on grain kinematics [38]. The final pattern of failure is encoded in the grain motions during the nascent stages of loading. DEM simulations [56,57] corroborate this aspect of localized failure. New work has revealed the possible structural origins of this early manifestation of failure, as well as the correspondence between boundary conditions, the development of vortex patterns, their evolution into shear bands, and the evolution of material fabric [57]. Among the outstanding problems that remain are: (a) an objective method for identification and characterization of vortices in 2D/3D kinematic vector fields, and (b) the development of a detailed understanding of their connection to energy transmission and the formation, and failure by buckling, of force chains.

A method for early detection of the ultimate mode of failure (i.e. localised versus diffuse) that a sample is likely to undergo was also recently developed using CS techniques [57] – without need for contact force information. This scheme relies only on contact information, while the study on sand relies on kinematical vector fields for input [38]. Could these new methods, which show great promise in the early detection of failure in laboratory scale samples, prove as effective in the analysis of ground motion data from real-time monitoring systems? In principle, the kinematic transmission scheme [37-38] should work for high-resolution ground motion data, and may aid studies of slope stability [58] and granular flows [59].

Complex networks of interstitial pores: Shear bands are deleterious to built environments but rich in pores that provide conduits for flow and recovery of petroleum and natural gas found in shale and tight rock formations [60]. Networks representing the coupled evolution of the grain matrix and their surrounding interstitial pore space have been studied. By tracking changes in the associated pore space, via the change in contact cycle topology around grains across a strain interval, a metric (CD) for the local change in energy was determined. When averaged across the assembly, CD correlates strongly with energy dissipation during failure. Percolating shortest paths in networks of pore space consistently go through the shear band [61] – in concordance with a recent multiscale DEM-Lattice Boltzman study [60]. Dilatancy inside shear bands not only increased porosity, but also led to a more interconnected pore space.

The response of earth structures during earthquakes was explored in recent earthquake centrifuge tests from the perspective of fabric evolution. Associated force chain evolution was implicated as the key mechanism behind the different liquefaction resistances observed for the various sand samples [62]. Yu and co-workers [62] highlight the need to take into account the micromechanics of force chains in future research into liquefaction and soil-structure interaction under seismic loading conditions.

Bridging the scales: dynamics from bulk time series data and grain scale measurements: As discussed in the first part, advances in acoustic emission (AE) are improving understanding of granular behavior across a range of spatial scales. A foundation for linking the transmission of acoustic emission energy with various micromechanical failure events in geologic granular materials was recently proposed for use in monitoring triggering events preceding slope failure from lab experiments to landslides in hill slopes and open pit mines [63]. Studies of geological hazards (e.g. rock debris [64], dense volcanic flows [59], ice rubbling [58], earthquakes [65] etc.), all aided by DEM simulations, show that mesoscopic force chains, regardless of breakage, provide the primary mechanism for load transfer, and their local failure by buckling governs failure and the attendant energy release at the macroscopic scale. In particular, a major challenge in large-scale applications is linking field observations (e.g. time series of bulk stresses) directly to force chains and meso-scale grain motions [29,58-59,62-63,66-67]. Thus new tools are needed that not only mine new insights on force chain dynamics, but can also tie these insights to the dynamics extracted from the real-time series data from field tests. In earthquake mechanics, attention has been paid to the connection between force chain dynamics and the dynamics of fault gouge using laboratory experiments involving photoelastic disks [68-69]. The principal output of such experiments is measured time series of bulk descriptors [65]. Tools from complex systems applied to time series including, but not limited to nonlinear signal processing [47,50-51,66-67] and complex networks [53,69-70] aid characterization of the underlying mechanisms responsible for stick-slip dynamics.

Improved knowledge of the relationship between internal processes and bulk data allow more realistic limits on predictability to be established. For example, in an experiment mimicking a propagating fault, periodic models were found to be insufficient, given a lack of evidence for long-term dynamical correlations between stick-slip cycles [69]. The material has no long-term memory. By contrast, in computer simulations mimicking a mature fault, results suggest that nonlinear models, possibly exhibiting chaos, could deliver short-term predictability of macroscopic behavior [70]. A key distinction between physical and virtual models of propagating versus mature faults, reflected in differences in the character of bulk measurements, is the subtle role of underlying force chain dynamics. The dynamics of a propagating fault is governed by newly born force chains which form and self-organize ahead of the propagating fault; the dynamics of a mature fault is governed by the re-organization of pre-existing force chain structures created from the previous deformation history of the fault.

Constitutive modeling and micromechanics

To this point, the focus has been upon the discrete nature of granular media, in particular on force-transmission and movement among the grains. Applying such grain-scale information to the study of large-scale boundary value problems usually requires a continuum description of the underlying discrete system. The unique mechanical behavior of granular materials derives from their grain-scale interactions and the manner in which these interactions influence the collective behavior of grains. Past studies on constitutive modeling of these materials were primarily based upon various phenomenological assumptions. However, the mathematical modeling of behavior based upon classical continuum approaches has posed special challenges. As has been described, recent technological advances in numerical and experimental tools have also enabled us to observe and capture the important role played by the discreteness of a granular system. Indeed there has been a wide recognition in recent years that continuum constitutive models should capture significant underlying mechanisms that occur at scales smaller than the representative volume element (RVE). The concepts of micro-mechanics, nano-mechanics, and multi-scale mechanics currently pervades modeling issues across all types of material systems. For granular materials, the interest is in discovering and characterizing how the interactions between particles influence the RVE behavior. This granular nature requires approaches that are different from the many micromechanical or multi-scale methods that have been conceived with the framework of continuum mechanics. Over the past three decades, granular micromechanics approaches have received increasing attention for continuum constitutive modeling. The state of art of research in constitutive modeling of granular media has now shifted to modeling approaches that are physically, micromechanically, and multiscale based. Three broad frameworks have been adopted in this modeling: an entirely continuum approach that can be calibrated to account for an evolving fabric; an upscaling approach in which the macro-scale continuum behavior is derived from grain interactions; and a multi-scale computational framework in which information at two scales, micro and macro, are shared in solving large boundary value problems.

Continuum constitutive modeling accounting for fabric and its evolution: Both experimental data and DEM simulations prove that fabric and its evolution affect the macro-scale behavior of granular materials [71,72]. Inspired by these observations, a recent trend has been to account for these fabric effects in constitutive models in a physically and thermodynamically consistent way. Along these lines, the theoretical framework of anisotropic critical state theories in geomechanics has been utilized to accommodate certain aspects of granular fabric [73-75]. Additional aspects of fabric, including the influence of the grain size distribution and its evolution due to grain breakage [76] or internal erosion [77] are being addressed in this framework. Other approaches that account for microstructural changes, especially related to long-term rate-effects have been proposed as enhancements to conventional theories [78]. The verifications and calibrations of these theories with respect to fabric evolution using experimental and/or numerical means remain a rich area of exploration. Other issues addressed with this approach span from unified descriptions of anisotropic elasticity and plasticity to comprehensive predictive frameworks for both monotonic and cyclic behaviors of sand, as well as their engineering applications for hazard mitigation (e.g. static and seismic liquefaction, flow slides, etc.).

Micromechanical constitutive models: from discrete to equivalent continua: The micromechanical approach utilizes homogenization paradigms to derive continuum constitutive models that explicitly incorporate the grain-interactions behavior [79,80]. In this approach, the inter-granular interactions are conceived in a statistical sense to describe the essential grain-scale and sub-granular scale mechanisms. The resultant models offer the versatility of investigating the influence of both the macro-scale parameters and the grain-scale parameters on the overall stress-strain response by incorporating the effect of meso-scale grain interactions through the inter-granular force-displacement relationship, orientation vectors, and average tensorial fabric measures. The advantages are clear since (1) the computational needs are far smaller than full-scale simulations with discrete particles, (2) the models naturally exhibit macro-scale effects such as volume-change and pressure sensitivity, and inherent and loading-induced anisotropy (fabric evolution) effects, and (3) the models can readily represent the micro-scale effects of particle interactions, including effects of degradation, presence of boundary layers, surface conditions, capillarity, particle shapes and sizes, stochastic nature of interactions, and loading rates. This approach has been applied to sands and grain-packing to include the representation of strength anisotropy [81] and the anisotropy of stress-dilatancy [82,83]; micro- and macro-scale instability analysis of sands [84] and rod assemblies [85]; the influence of fines [86-88]; and cyclic behavior [89]. Significant recent developments have been concerned with the introduction of various physical phenomena at the particle scale, such as damage in cemented granular materials [90,91], the additional forces at particle contacts produced by capillarity in unsaturated materials [92], and surface energy forces [93]. The evolution of granular media with time is also an area of on-going research and concerns various phenomena such as internal erosion [94], physico-chemical degradation, creep and loading rate-effects [95,96]. Issues related to thermodynamic consistency of these models [80] and the modeling of higher-order effects [97] are also receiving attention with this approach.

Computational multiscale models: Computational multiscale approaches based upon the scale-bridging concept have attracted considerable recent attention in material science (see among others [98,99]). For granular media, recent efforts along these lines have focused upon incorporating a two-scale macro-micro hierarchical structure into a computational modeling framework [75,100,101]. This hierarchical multiscale approach for granular media typically employs a rigorous coupling between the finite element method (FEM) for the macro domain and the Discrete Element Method (DEM) for the micro scale, rendering an effective scale bridging (Fig. 2). This approach avoids the phenomenological nature of conventional continuum constitutive modeling by seeking to directly link the macroscopic observations, modeled in terms of continuum variables, to the underlying micromechanical mechanisms at the material point (i.e., an integration point in the FE model) which is simulated through discrete particle models whose behavior is governed by inter-particle contact laws. Thus the constitutive model that is used in the FE calculations is provided by DEM simulations of a pre-specified particle model. The hierarchical structure also exploits the implementation of distributed parallel computing for solving large-scale boundary value problems. The computational issues raised by this approach have received recent attention, such as efficiently incorporating experimentally acquired information into the multiscale framework to render accurate predictions (Fig. 2) [102-104].

Discrete computational modeling

Much has already been mentioned about the discrete computational modeling of granular materials, in which a material region is explicitly modeled as a collection of discrete grains. The discrete element method (DEM) was the earliest of these methods, and because of its versatility and adaptability, it is currently the prevailing computational approach, although other methods are also being used to effectively explore granular behavior (e.g., the contact dynamics (CD) method and discontinuous deformation analysis (DDA)). Developments in DEM have followed a pattern in which new extensions of the method (new particle shapes, new contact models, new particle-body models) are rapidly followed by their exploitation in exploring new behaviors that had previously defied understanding. The method is now most useful for modestly large assemblies of hard durable particle that interact at discrete contact points by employing simple force-displacement rules. In spite of numerous advances in modeling methodologies and computing power, the DEM method is still limited to a relatively small range of problems and faces significant obstacles for its application to a wider breadth of important, practical problems in geomechanics and materials processing. We briefly review some of these challenges and advances in the modeling of such realistic problems.

Particle shape, durability, and size: Abundant evidence is now available on the importance of particle shape and surface texture to the bulk characteristics of dense granular materials. Of particular consequence are the presence of sharp corners and edges and the con-convexity of particle bodies. Particle shapes have been progressively generalized to include polyhedra, bonded-sphere and overlapped-spheres clusters, super-quadrics, and composites of spheres, ellipsoids, tori, and spline surfaces, so that realistic grain shapes can now be modeled [105-107]. Recently, non-spherical elements, such as polyhedral, spherocylinder, circular plate, spheropolygon and platy particles have been constructed based on Minkowski sums to accurately model realistic complex particles [108-110]. With these irregular-shaped particles, the mechanical behaviors of concrete, railway ballast, ice floes, and textured industrial powders can be modeled more realistically. Although these methods have been assisted by developments in computed tomography (CT) to capture the shapes and arrangements within particle assemblies, there is a palpable need for more efficient codes to simulate complex grain shapes for a large number of particles during extended deformation and flow. Besides the geometric modeling of a particle's shape, one must also code an efficient algorithm for detecting a particle’s contacts (or lack of contact) with surrounding particles. Contact detection is a key element affecting DEM computational efficiency [111]. A fast contact detection technique based on tree-codes can enhance DEM applications on industrial scale, especially for non-spherical particles.

Many granular materials are loaded to levels that produce crushing, chipping, and gouging of particles: geomaterials at extended depths, friable powders, and powder compacts in which particle crushing is not just expected but is intentional and desired. Indeed, the largest industrial operations – mining, mineral extraction, and aggregate production – are essentially grain crushing (comminution) efforts on a massive scale. In geomaterials, the plastic volumetric response is largely a result of particle breakage, and the realistic simulation of granular behavior at stresses greater than a few atmospheres requires the inclusion of non-durable, breaking particles and the inclusion of a rational particle fracture criterion. When the granular mass is experiencing severe fragmentation, a continuum finite element analysis certainly fails to capture this micro-scale phenomenon. Although microstructural fracture mechanics (MFM) holds some promise, it requires a damage criteria and parameters, not to mention the unrealistic computation times associated with even small problems. Several approaches have been developed recently for discrete modeling in this regard: particles modeled as multiple geometric objects that can separate with sufficient loading, and finite-discrete (FDEM) particles modeled as numerically fused continuum blocks [112]. By considering the inter-particle bond-breaking effect of polyhedral elements, the fracture of grain continua can also be simulated [110]. New methods and advances of these and other promising methods are greatly needed by industrial and geotechnical engineers.

Current DEM algorithms also favor the modeling of granular assemblies that contain a narrow distribution of particle sizes, and simulations with a size range greater than 20 are rare. The limitation stems from the necessity of a time step that is controlled by the smallest particle within an assembly, as well as by predominance in the number of the smallest particles. This limitation essentially precludes the modeling of many geomaterials and friable powders: a silty gravel is simply beyond the capability of most codes. Novel methods for modeling these materials (perhaps using multi-scale methods) are now of intense interest.

At the other extreme of particle durability, materials composed of soft, highly deformable grains, such as colloidal gels, gel tablets, and dispersed bubble flows have received scant attention and are still awaiting systematic investigation with DEM and other discrete micromechanical models.

Grain interactions: Although recent advances in discrete modeling have been focused on grain shape, size, and strength, an appropriate modeling of particle interactions is equally important. Most DEM models represent the particles as having glassy smooth surfaces in which the interactions are either through linear springs or simplified Hertz-Mindlin models. A full Hertz-Mindlin representation that respects all possible sequences of contact motions is quite complex [113], but this representation, although computationally taxing, is but a simplification of the more complex interactions between textured particles surfaces. Recent experimental measurements of the interactions of silicate grains reveal unusual behaviors that have not been precisely replicated in discrete models [114,115]. Moreover, micro-graphs of polished thin-sections as well as CT images reveal that the particles of geomaterials do not simply touch at isolated point, but contact at multiple points or are fully nestled together.

Although particle interactions are usually modeled as contact springs that transmit moments as well as forces, these simple phenomenological models belie the underlying complexity of real materials. For instance, as grains become sufficiently small or become wet enough, adhesion phenomena, which are insignificant at larger scales, begin to become important [116]. The significance of adhesion also depends on the magnitude of the applied load and on the roughness and cleanliness of the surfaces. Atomic force microscopy (AFM) is now being used to determine the interparticle surface energy and properties related to rolling and sliding friction in the presence of adhesion, for inclusion in DEM computations [117]. Within the context of DEM, we typically assume that adhesive forces due to van der Waals interactions between particle act on length scales that are much smaller than the particle size, such that, in most cases, classic adhesive contact models, e.g., JKR, DMT, etc., have been incorporated into DEM simulations by using a multi-time scale approach [118,119]. Apart from normal adhesive contacts, the energy dissipation mechanisms related to sliding, rolling, and twisting frictions in the presence of adhesion can also be incorporated into DEM. Such simulations can be validated by particle-wall impact, singer-fiber deposition experiments, etc. The treatment of long-range capillary forces between particles, which typically act on a scale comparable to the particle diameter, is still not mature and deserves future attention. Other long-range interactions that can predominate among small particles include electrostatic and double-layer forces. Recently, a computational approach for simulating electric fields in conjunction with DEM was established, by introducing the fast multipole method (FMM) and the boundary element method (BEM) to accounting for electric fields induced by particles and macroscopic bodies, respectively [120].

We note that, unlike most current modeling, we should no longer accept uniform values for any of the above mentioned particle or contact properties. It has been shown, for example, that soils are composed of individual grains that vary in shape, size, surface roughness, stiffness, local void distributions, etc. Therefore, realistic distributions of these properties should be employed in realistic discrete models.

Numerical reconstruction from image analysis: Besides capturing the shapes, sizes, and strengths of particles, the bulk behavior can be markedly affected by the details of their arrangement. Image processing using mathematical morphology allows one to reconstruct both the particle solids and the void space, although high resolutions are required for distinguishing the contacts between particles.

An interesting application of these methods to discrete numerical modeling is the simulation of asphalt cement concretes, which are composed of hard stone grains with a binder matrix and air that fill the void space. Image-based models of asphalt concrete are becoming widely used because they can accurately capture the component phases of these exceedingly complex materials. Image processing techniques are now used to discriminate aggregate particles and air voids within an asphalt matrix. The limitation of image-based modeling is that it is time consuming and expensive. To solve this issue, some user-defined models have been developed as an alternative. The essential aspect of these models is creating numerical representatives for component phases of an asphalt mixture in a user-defined algorithm. In the past, user-defined models were simplified, often with aggregate particles of simple shapes, and uniformly distributed air voids. Recently, researchers have been creating numerical models more comparable to the realistic materials. Techniques such as X-Ray CT and aggregate imaging system (AIMS) have been utilized to produce numerical representatives of realistic aggregate particles [121-123]. Researchers have also been making efforts to establish representative libraries of aggregate particles having a range of different shapes and angularities [124], so that users can generate realistic numerical assemblies by invoking representatives from the libraries.

Interactions between granular materials and structures: The DEM and finite element method (FEM) are now being combined to model the interactions between particles and engineering structures and the fracture process of continuum materials at two different scales. Structures are modeled with FEM at the macro scale, and the granular material is simulated with DEM at the micro scale. In a DEM-FEM coupling model, the interaction forces between particles and structures must be specified exactly, although the computational time steps of the two models are quite different. Because the locations of the contact points change rapidly, due to particle motions, it is necessary to frequently search the contact locations in local and global coordinates, respectively [125]. Moreover, the node-to-surface contact detection algorithm must also be adopted to determine the contact location [126]. To determine the contact force at the DEM-FEM interface, the contact forces at each node of the FEM structure can be calculated based on shape functions [125,127]. Moreover, a plenary function has also developed to determine the contact force [126,128]. Most recent investigations apply spherical particles in DEM-FEM models. The modeling becomes far more complex if the particles are constructed with irregular shapes, which may have multiple contact points with an element of the structure.

Parallelized simulations: To simulate granular behavior with greater efficiency, especially with realistic, large-scale problems, parallel computations with multi-CPU (central processing unit) and GPU (graphics processing unit) techniques are being rapidly developed for fast neighbor searching and contact detection in DEM simulations [129,130]. For irregular particle shapes, contact detection and contact force calculations are more complex than those for spherical elements, but the computational scale and efficiency can also be improved significantly with GPU-based parallel computations. For more complex granular systems with CFD-DEM-FEM coupling, high performance numerical algorithms must be improved to solve complicated but important problems.

Part III. Multi-phase Modeling

In both natural environments and industrial processing, granular materials are often multi-phase materials, in which interactions occur among the solid grains, within the fluid continuum, and between the solid and fluid phases. For decades, the coupled response of multi-phase systems has attracted research in related phenomena, such as consolidation, poroelasticity and fluidization. Early studies relied on phenomenological approaches based on the continuum mechanics of mixtures. In this view, a granular material is considered to be a superposition of two (and possibly more) continuous media (representing the phases) with energy exchanges and restrictions imposed by interactions among the phases. Recent research efforts are instead based on an amalgam of continuum-discrete and discrete approaches [131] in which the solid phase is modeled using the discrete element method (DEM). For low moisture content, the lubrication and suction associated with pore fluid are modeled using appropriate inter-particle contact laws and forces, which have been used to study topics ranging from the effect of wetting and drying cycles on unsaturated soils (e.g., [132]) to the influence of interstitial water on stress conditions [133].

In a fully saturated material, the presence of fluid phases in the pores requires special treatment. The current state of coupling the fluid and particles utilizes a continuum description of the fluid phase(s) using an averaged form of Navier-Stokes equations. While a continuum description of the fluid appears to be satisfactory, it does not allow for a fundamental investigation of the actual interaction between the pore-fluids and the solid particles. Motivated by an upsurge in computational power, recent work in fluid-particle coupling attempts to model the fluid at the pore-scale. This type of coupling has no empiricism at any level, and two approaches, described below, are now being used to model solid-fluid interactions.

Continuum-Scale modeling of fluid phase

The pore-fluid can be modeled at a macro-scale using volume-averaged Navier-Stokes equations. These are the transient mass and momentum balance equations of the flowing fluid taking into consideration that the fluid only occupies the pore voids of the granular media. The interphase momentum transfer accounts for the dynamic change in porosity and possible occurrence of nonlinear losses. This approach was originally developed by Tsuji and co-workers for modeling fluidized beds [134]. The fluid particle interaction term that presents momentum transfer is a function of the forces applied by the fluid on the particles, which include drag forces and lift-off forces. The shear lift originates from the inertia effects in the viscous flow around the particle and is important in problems such as surface erosion. Lift is a function of relative fluid-particle velocity, shear rate, particle diameter, and the density and viscosity of the fluid. On the other hand, the drag force reflects the frictional energy dissipated through interaction between the flowing fluid and the surface of solid particles, and it is a function of packing density, relative fluid-particle velocity, particle diameter, and fluid viscosity.

The use of an average description to model the fluid is the most efficient and practical way to model coupled fluid-particle problems. It can be employed for a wide range of applications such as water flow in a deforming porous media [135], liquefaction [136], fluidization of particle beds (e.g., [134]), among others. Unlike some continuum models, the averaged Navier-Stokes equations do not need a special mechanism for pore-pressure buildup for modeling problems such as soil liquefaction.

Pore-Scale modeling of fluid phase

Other coupled techniques can model fluid flow at the pore-scale. Such techniques are capable of obtaining the actual fluid flow pattern in the pore space between particles. Patankar et al. [137] used a finite element technique based on moving unstructured grids to study the lift force on a single particle and on multiple particles. A two-dimensional generalized Galerkin finite element formulation which incorporates both the fluid and particle equations of motion into a single variational equation was used for Newtonian fluids. An arbitrary Lagrangian-Eulerian technique was adopted to deal with the motion of particles inside the fluid domain. At each time step, particle positions and mesh nodes were updated. If unacceptable element distortion was detected, a new finite element grid was generated via a remeshing technique. This system of fluid and moving particles requires continual remeshing which significantly increases the computational cost.

Zhu et al. [138] implemented the Smoothed Particle Hydrodynamics (SPH) method to investigate the flow through stationary porous media. SPH is a fully Lagrangian technique in which the solution is obtained without a grid (meshless). In this technique, the fluid velocity and pressure can be obtained at the pores. Potapov et al. [139] and Cleary et al. [140] combined SPH and DEM to simulate liquid-solid flows. Arbitrary boundary conditions and free surface problems can be modeled well with SPH approach. This coupling approach has been applied in rock blasting, fluidized beds and geomechanics, etc.

The lattice Boltzmann method (LBM) is an alternative numerical technique to simulate fluid flow governed by Navier-Stokes equations. LBM is based on the microscopic kinetic equation for the fluid particle distribution function. The macroscopic quantities are then obtained through momentum integration of the distribution function. LBM models fluid flow at a mesoscale and the fluid characteristics are obtained within the pore space. Moreover, the forces in LBM are calculated based on the stresses applied to the particles or the momentum that the fluid exchanges with the particles. With the availability of very fast and massively parallel machines, there is a current trend to use codes that can exploit high-performance parallel and distributed computing. With its explicit computing algorithms that generally require information in the immediate vicinity of a fluid node, LBM fulfills these requirements in a straightforward manner compared to other techniques such as SPH. Coupled LBM-DEM models have been used to study a wide range of problems such as liquefaction [141], surface erosion [142,143], and particulate suspensions [144].

All of these pore-scale techniques are essentially for a continuum, but they possess the capability of reaching the pore-scale to model fluid in the void space between particles. These techniques can seamlessly handle particles of irregular shape. The methods have even be used to model the flow behavior of highly viscid asphalt mixtures during mixing, simulating aggregate heating in asphalt plants through the coupling of CFD and DEM [145]. Future research in modeling fluid-particle interaction should focus on developing algorithms that efficiently link the solid particles to fluid nodes in their immediate vicinity to minimize search algorithms during the application of boundary conditions at the particle-fluid interface. Furthermore, models that incorporate a rigid or flexible structural element that interacts with the fluid-particle system need to be developed. New trends should also generalize the formulation to include three-phase systems (solid particles, gas, and liquid).

Coupled thermo-hydro-mechanical-chemical processes

The presence of a heat source or an influx of thermal energy within a granular material, such as soil, leads to a coupled thermal-hydro-mechanical (THM) response. This response involves moisture and heat flow concurrent with deformation of the granular skeleton, and it plays an important role in a number of applications that include nuclear waste repositories, underground power lifelines, and geothermal systems. In addition to the usual hydro-mechanical coupling (described above), heat introduces another level of complexity associated with thermally induced moisture (liquid and vapor) flow in soils and also moisture phase transitions that require rigorous thermodynamic analysis and modeling tools. Motivated by a need for safe nuclear waste repositories, the noteworthy international collaboration DECOVALEX project was initiated in 1992 to advance the understanding of THM processes in geologic systems [146]. A number of other studies [147] and associated computational codes are being used to address this topic using phenomenological continuum approaches. Other applications include CO_2 storage [148] and geothermal field studies [149]. Some more recent studies employ a discrete approach that relies on the use of the DEM along with a network of heat (particle) reservoirs and thermal contacts [150]. Such thermal modeling may then be coupled with a hydro-model in which pore fluid flows through another associated network of channels and reservoirs to study, for instance, the process of rock hydraulic-fracturing (fracking) [151].

The water phase of granular media generally includes minerals that may lead to oxidation-reduction, crystallization, precipitation, sorption or deposition, which affects the physical and mechanical properties of these media. These hydro-mechanical-chemical (HMC) mechanisms may involve chemical processes that occur naturally or are affected by biological activities (i.e., action of micro organisms). In turn, the chemical and biological processes can significantly affect the soil porosity, compressibility, strength and other properties and are being proposed a tools for remediation and restoration and retrofitting of soil systems (i.e., against seismic activities or erosion). The idealization of these various phenomena requires models to describe the following: (1) the processes of chemo- and bio- reactions and grouting within saturated and unsaturated deformable porous medium, and (2) the consequences and effects on the solid matrix composition and mechanical properties. These phenomena were addressed by a number of researchers using continuum mechanic (e.g., [152,153]). In contrast, Yasuhara [154] used a discrete approach. In this approach, minerals dissolve at the inter-particle contacts of a granular medium owing to highly localized stresses and the precipitation that occurs along the free faces of pore walls. These mechanisms were used to assess their affect on particle size, and, thus porosity and permeability [155].

The realistic idealization of the different THMC processes of a granular medium and their interactions using a single model is a complicated undertaking. Such a model requires the integration of a number of dissimilar processes over different space and time scales. Discrete and continuum-discrete models, which reflect the particulate nature of granular media, are increasingly employed to addresses some of the associated complexities. These models are mechanistic, idealize directly the particle-level phenomena dictating the macro scale response, and are consequently often simpler to formulate than phenomenological ones. With proper parameterization, the mechanistic models have reduced the need for parameters obtained from experimentation. These models are becoming more popular as they provide valuable tools to explore and explain a number of underlying phenomena that constitute a challenge based solely on observations. This is especially true for extreme conditions such as large deformations and failure. However, discrete and continuum-discrete models generally necessitate large computational resources and may require coarse-grained discretization. These models are generally practical only for small boundary value problems, and as such will remain for a while a research instrument more than a routine simulation and analysis tool. Nevertheless, discrete models provide valuable means to supplement and possibly improve continuum phenomenological formulations.

Conclusion

The paper has summarized recent trends in granular mechanics, and although much progress has been made, the future abounds with significant, and in some cases seeming insurmountable, challenges. These challenges arise in developing new experimental and imaging methodologies; in developing and exploiting new methods for extracting meaning from the resulting micro-scale data; in applying an understanding of the micro-scale to develop general, realistic continuum models for effectively analyzing and solving engineering problems; in developing new computational techniques and efficiencies that can confront large-scale modeling problems; and in extending single-phase models toward multi-phase models and multi-phenomena models that will be required to solve the most difficult problems in geomechanics, mining, and materials processing.

References

[1] Hammad, T. (2010). "Behaviour of deepwater marine sediments : a multiscale approach [Comportement des sédiments marins de grande profondeur : approche multiéchelle]", Doctoral dissertation (in french), Ecole Centrale Paris, France.

[2] Hattab, M., and Fleureau J. M. (2010). “Experimental study of kaolin particle orientation mechanism.” *Géotechnique*, 60(1), 323-331.

[3] Hattab, M., and Hammad, T., Fleureau, J-M., Hicher, P-Y. (2013). “Behaviour of a sensitive marine sediment: microstructural investigation.” *Géotechnique*, 63(1), 71-84.

[4] Delage, P. (2010). “A microstructure approach to the sensitivity and compressibility of some Eastern sensitive clays.” *Géotechnique*, 60(5), 353-368.

[5] Adelinet, M., Fortin, J., Schubnel, A., and Guéguen, Y. (2013). “Deformation modes in an Icelandic basalt: From brittle failure to localized deformation bands.” *J. of Volcanology and Geothermal Res.*, 255, 15-25.

[6] Le Gonidec Y., Schubnel A., Wassermann J., Gibert D., Nussbaum C., Kergosien B., Sarout J., Maineult A., and Guéguen Y. (2011). “Field-scale acoustic investigation of a damaged anisotropic shale during a gallery excavation.” *Int. J. of Rock Mech. and Mining Sciences*, 51, 136-148.

[7] Andò, E., Viggiani, G., Hall, S., and Desrues, J. (2013). “Experimental micro-mechanics of granular media studied by x-ray tomography: Recent results and challenges.” *Geotechnique Lett.*, 3, 142-146.

[8] Gilbert, A. J., and Deinert, M. R. (2013). “Neutron tomography of axisymmetric flow fields in porous media.” *Nuclear Instruments and Methods in Physics Res. B*, 301, 23–28.

[9] Daouadji, A., and Jrad, M. (2011). French patent FR1161654 “Device for performing biaxial tests on granular materials and powders.”

[10] Radjaï , F., Jean, M., Moreau, J.-J., and Roux, S. (1996). “Force distributions in dense two-dimensional granular systems.” *Phys. Rev. Lett.*, 77(2), 274-277.

[11] Kuhn, M. R. (1999). “Structured deformation in granular materials.” *Mech. of Mater.*, 31(6), 407-429.

[12] Radjaï , F., and Roux, S. (2002). “Turbulentlike fluctuations in quasistatic flow of granular media.” *Phys. Rev. Lett.*, 89(6), 064302.

[13] Thornton, C. (2000). “Numerical simulations of deviatoric shear deformation of granular media.” *Géotechnique*, 50(1), 43–53.

[14] Gilabert, F., Roux, J.-N., and Castellanos, A. (2007). “Computer simulation of model cohesive powders: Influence of assembling procedure and contact laws on low consolidation states.” *Phys. Rev. E*, 75(1), 011303.

[15] Tordesillas, A., and Walsh, D. C. S. (2002). “Incorporating rolling resistance and contact anisotropy in micromechanical models of granular media.” *Powder Technol.*, 124(1-2), 106-111.

[16] Estrada, N., Taboada, A., and Radjaï, F. (2008). “Shear strength and force transmission in granular media with rolling resistance.” *Phys. Rev. E*, 78(2), 021301.

[17] Azéma, E., Radjai, F., and Dubois, F. (2013). “Packings of irregular polyhedral particles: Strength, structure, and effects of angularity.” *Phys. Rev. E*, 87(6), 062203.

[18] Wegner, S., Stannarius, R., Boese, A., Szabo, B., Somfai, E., and Börzsönyi, T. (2014). “Effects of grain shape on packing and dilatancy of sheared granular materials.” *Soft Matter*, 10, 5157-5167.

[19] Ueda, T, Matsushima, T., Yamada, Y. (2013). “DEM simulation on the one-dimensional compression behavior of various shaped crushable granular materials.” *Granular Matter*, 15(5), 675-684.

[20] Peyneau, P.-E., and Roux, J.-N. (2008). “Frictionless bead packs have macroscopic friction, but no dilatancy.” *Phys. Rev. E*, 78(1), 011307.

[21] Lemaître, A., Roux, J.-N., and Chevoir F. (2009). “What do dry granular flows tell us about dense non-Brownian suspension rheology?” *Rheologica Acta*, 48(6), 925-942.

[22] Forterre, Y., and Pouliquen, O. (2008). “Flows of dense granular media.” *Annual Rev. of Fluid Mech.*, 441, 727-730.

[23] Staron, L., Lagrée, P.-Y., and Popinet, S. (2014). *European Phys. J. E*, 37:5.

[24] Agnolin, I., and Roux, J.-N. (2007). “Internal states of model isotropic granular packings. I. Assembling process, geometry, and contact networks.” *Phys. Rev. E*, 76(6), 061302.

[25] Roux, J.-N. and Combe, G. (2002). “Quasistatic rheology and the origins of strain.” *Comptes Rendus Physique*, 3(2), 131–140.

[26] Radjaï, F., and Richefeu, V. (2009). “Contact dynamics as a nonsmooth discrete element method.” *Mech. of Mater.*, 41(6), 715–728.

[27] McNamara, S., and Herrmann, H. J. (2006). “Quasirigidity: Some uniqueness issues.” *Phys. Rev. E*, 74(6), 061303.

[28] Welker, P. R., and McNamara, S. C. (2009). “What triggers failure in frictional granular assemblies?” *Phys. Rev. E*, 79:061305.

[29] Rechenmacher, A., Abedi, S., and Chupin, O. (2010). “Evolution of force chains in shear bands in sands.” *Géotechnique*, 60, 343-351.

[30] Bi, D., Zhang, J., Chakraborty, B., and Behringer, R.P. (2011). “Jamming by shear.” *Nature*, 480, 355-358.

[31] Cil, M., and Alshibli, K. (2012). “3D assessment of fracture of sand particles using Discrete Element Method.” *Geotechnique Lett.*, 2, 161-166.

[32] Ottino, J.M. (2011). “Chemical engineering in a complex world: grand challenges, vast opportunities.” *AICHE J.*, 57, 1654-1668.

[33] Arevalo, R., Zuriguel, I., and Maza, D. (2010). “Topology of the force network in the jamming transition of an isotropically compressed granular packing.” *Phys. Rev. E*, 81, 041302.

[34] Walker, D.M., and Tordesillas, A. (2010). “Topological evolution in dense granular materials: A complex networks perspective.” *Int. J. of Solids and Structures* 47, 624-639.

[35] Tordesillas, A., O’Sullivan, P., Walker, D.M., Paramitha (2010). “Evolution of functional connectivity in contact and force chain networks: feature vectors, k-cores and minimal cycles.” *Comptes-Rendus Mecanique*. *Proc. of the French Academy of Sciences* 338, 556-569.

[36] Danielle, S.B., Owens, E.T., Daniels, K.E., and Porter M.A. (2012). “Influence of network topology on sound propagation in granular materials” *Phys. Rev. E*, 86, 041306.

[37] Walker D.M., Tordesillas A, Pucilowski S, Lin Q, Rechenmacher A, Abedi S (2012) “Analysis of

grain-scale measurements of sand using kinematical complex networks" *Int. J. of Bifurcation and Chaos*, 22, 1230042.

[38] Tordesillas, A., Walker, D.M., Andò, E., and Viggiani, G. (2013). "Revisiting localized deformation in sand with complex systems." *Proc. of the Royal Soc. of London Series A*, 469, 1471-2946.

[39] Lin, Q., Tordesillas, A. (2014). "Towards an optimization theory for deforming dense granular materials" *J. of Industrial and Management Optimization*, 10, 337-362.

[40] Tordesillas, A., Lin, Q., Zhang, J., Behringer, R.P., Shi, J. (2011) "Structural stability and jamming of self-organized cluster conformations in dense granular materials" *J. of the Mech. and Physics of Solids* 59, 265-296.

[41] Tordesillas, A., Walker, D.M., and Lin, Q. (2010). "Force cycles and force chains." *Phys. Rev. E*, 81, 011302.

[42] Tordesillas, A., Walker, D.M., Froyland, G., Zhang, J., and Behringer, R. (2012). "Transition dynamics and magic-number-like behavior of frictional granular clusters." *Phys. Rev. E*, 86, 011306.

[43] Tordesillas, A., Pucilowski, S., Sibille, L., Nicot, F., Darve, F. (2012). "Multiscale characterisation of diffuse granular failure." *Philosophical Mag.*, 92, 4547-4587.

[44] Wang, X., Zhu, H., Luding, S., and Yu, A.B. (2013). "Regime transitions of granular flow in a shear cell: A micromechanical study." *Phys. Rev. E*, 88, 032203.

[45] Milo, R., Shen-Orr S.S., Itzkovitz, S., Kashtan, N., Chklovskii, D., Alon, U. (2002). "Network motifs: simple building blocks of complex networks." *Science*, 298, 824–827.

[46] Walker, D.M., Tordesillas, A., Zhang, J., Behringer, R.P., Ando, E., Viggiani, G., Druckrey, A., and Alshibli, K. (2014). "Structural templates of disordered granular media." *Int. J. of Solids and Structures* (in press).

[47] Walker, D.M., Tordesillas, A., Ren, J., Dijskman, J., and Behringer, R.P. (2014) "Uncovering temporal transitions and aging dynamics in granular materials under cyclic shear using quadrant scans." *Europhysics Lett.*, 107, 18005.

[48] Peters, J., and Berney, E. (2010). "Percolation threshold of sand-clay binary mixtures." *Journal of Geotechnical and Geoenvironmental Engrg.*, 136, 310-318.

[49] Burnley, P.C. (2013). "The importance of stress percolation patterns in rocks and other polycrystalline materials." *Nature Communications*, 4, 3117.

[50] Xiang, R., Zhang, J., ke Xu, X., and Small, M. (2012). "Multiscale characterization of recurrence-based phase space networks constructed from time series." *Chaos*, 22, 013107.

[51] Rapp P E., Darmon D.M., and Celluci C. J. (2013). International Symposium on Nonlinear Theory and its Applications, NOLTA2013, Santa Fe, USA, September 8–11 2013, IEICE Proceedings Archive (IEICE) 2013, p. 286.

[52] Tordesillas, A., Steer, C.A.H., and Walker, D.M. (2014). "Force chain and contact cycle evolution in a dense granular material under shallow penetration." *Nonlinear Processes in Geophysics, Special Issue: Complex network approaches to analyzing and modeling nonlinear systems in geosciences*. 21, 505-519.

[53] Tordesillas, A., Hilton, J., and Tobin, S. (2014) "Stick-slip and force chain evolution in a granular bed in response to a grain intruder." *Phys. Rev. E*, 89, 042207.

[54] Butlanska, J., Arroyo, M., Gens, A., and O'Sullivan, C. (2013). "Multi-scale analysis of cone penetration test (CPT) in a virtual calibration chamber." *Canadian Geotech. J.*, 51, 51-66.

[55] Padbidri, J.M., Hansen, C.M., Mesarovic, S.D., and Muhunthan, B. (2012) "Length scale for transmission of rotations in dense granular materials." *J. of Applied Mech.*, 79, 031011.

[56] Peters, J., and Walizer, L. (2013). "Patterned nonaffine motion in granular media." *J. of Engrg. Mech.*, 139, 1479–1490.

[57] Tordesillas, A., Pucilowski, S., Walker D.M., and Peters, J., and Walizer, L. (2014). "Micromechanics of vortices in granular media: connection to shear bands and implications for continuum modelling of failure in geomaterials." *Int. J. of Numerical and Anal. Methods in Geomechanics*, 38, 1247-1275.

[58] Paavilainen, J., and Tuhkuri, J. (2013). "Pressure distributions and force chains during simulated ice rubbling against sloped structures." *Cold Regions Science and Technology*, 85, 157–174.

[59] Estep, J., and Dufek, J. (2013). "Discrete element simulations of bed force anomalies due to force

chains in dense granular flows." *J. Volcanology and Geothermal Res.*, 254, 108–117.

[60] Sun, W.C., Kuhn, M.R., and Rudnicki, J.W. (2013). "A multiscale DEM-LBM analysis on permeability evolutions inside a dilatant shear band." *Acta Geotechnica*, 8, 465-480.

[61] Walker, D.M., Vo, K., and Tordesillas, A. (2013). "On Reynolds' Dilatancy and Shear Band Evolution: A New Perspective." *Int. J. of Bifurcation and Chaos*, 23, 1330034.

[62] Yu, H., Zeng, X., Li, B., and Ming, H. (2013). "Effect of fabric anisotrophy on liquefaction of sand." *J. of Geotech. and Geoenvironmental Engrg.*, 139, 765–774.

[63] Michlmayr, G., Cohen, D., and Or, D. (2012). "Sources and characteristics of acoustic emissions from mechanically stressed geologic granular media — A review." *Earth Science Reviews*, 112, 97-114.

[64] De Blasio, F.B., and Crosta, G.B. (2014). "Simple physical model for the fragmentation of rock avalanches." *Acta Mechanica*, 225, 243-252.

[65] Daub, E.G., and Carlson, J.M. (2010). "Friction, fracture, and earthquakes." *Annual Rev. of Condensed Matter Phys.*, 1, 397–418.

[66] Walker, D.M., Tordesillas, A., Nakamura, T., and Tanizawa, T. (2013). "Directed network topologies of smart grain sensors." *Phys. Rev. E*, 87, 032203.

[67] Walker, D.M., Tordesillas, A., and Rechenmacher, A.L. (2013). "Transmission of kinematic information in dense granular systems: local and nonlocal network sensing." *Acta Geotechnica*, 8, 547-560.

[68] Hayman, N.W., Ducloué, L., Foco, K.L., and Daniels, K.E.D. (2011). "Granular controls on periodicity of stick-slip events: kinematics and force-chains in an experimental fault." *Pure and Appl. Geophysics*, 168, 2239-2257.

[69] Walker DM, Tordesillas A, Small M, Behringer RP, Tse CK (2014). "A complex systems analysis of stick-slip dynamics of a laboratory fault." *Chaos*, 24, 013132.

[70] Small, M., Walker D.M., Tordesillas, A., Tse, C.K. (2013). "Characterizing chaotic dynamics from simulations of large strain behavior of a granular material under biaxial compression." *Chaos*, 23, 013113.

[71] Li, X. S, and Li, X. (2009). "Micro–macro quantification of the internal structure of granular materials." J. *of Engrg. Mech.*, ASCE, 135(7), 641-656.

[72] Guo, N, and Zhao, J. (2013). "The signature of shear-induced anisotropy in granular media." *Computers and Geotechnics*, 47, 1-15.

[73] Li, X. S., and Dafalias Y. F. (2013). "Anisotropic critical state theory: the role of fabric." *J. of Engrg. Mech.*, ASCE, 138(3), 263-275.

[74] Zhao, J., and Guo, N. (2013). "Unique critical state characteristics in granular media considering fabric anisotropy." *Géotechnique*, 63(8), 695-704.

[75] Guo N., and Zhao J. (2014). "A coupled FEM/DEM approach for hierarchical multiscale modelling of granular media." *Int. J. for Numerical Methods in Engrg.*, 99(11), 789-818.

[76] Daouadji, A., and Hicher, P.-Y. (2010). "An enhanced constitutive model for crushable granular materials." *Int. J. Numerical and Anal. Methods in Geomechanics*, 34(6), 555-580.

[77] Scholtès, L., Hicher, P.-Y., and Sibille, L. (2010). "Multiscale approaches to describe mechanical responses induced by particle removal in granular materials." *CRAS Mécanique*, 338(10).

[78] Darabi, M. K., Abu Al-Rub, R. K., Masad, E. A., Huang, C.-W., and Little, D. N. (2012). "A modified viscoplastic model to predict the permanent deformation of asphaltic materials under cyclic-compression loading at high temperatures." *Int. J. of Plasticity*, 35, 100-134.

[79] Chang, C. S., and Hicher, P.-Y. (2005). "An elasto-plastic model for granular materials with microstructural consideration." *Int. J. of Solids and Structures*, 42(14), 4258-4277.

[80] Misra, A. and Singh, V. (2014). "Thermomechanics based nonlinear rate-dependent coupled damage-plasticity granular micromechanics model." *Continuum Mech. and Thermodynamics*, (doi: 10.1007/s00161-014-0360-y)

[81] Chang, C. S, and Yin, Z.-Y. (2010a). "Micromechanical modelling for inherent anisotropy in granular materials." *J. of Engrg. Mech.*, ASCE, 136(7), 830-839.

[82] Chang, C. S., and Yin, Z.-Y. (2010b). "Modeling stress-dilatancy for sand under compression and extension loading conditions." *J. of Engrg. Mech.*, ASCE, 136(6), 777-786.

[83] Yin, Z.-Y., and Chang, C. S. (2013). "Stress-dilatancy behavior for sand under loading and unloading conditions." *Int. J. for Numerical and Anal. Methods in Geomechanics*, 37(8), 855-870.

[84] Chang, C. S, Yin Z.-Y., and Hicher, P. Y. (2011). "Micromechanical analysis for inter-particle and assembly instability of sand." *J. of Engrg. Mech.*, ASCE, 137(3), 155-168.

[85] Misra, A., and Poorsolhjouy, P. (2014). "Micro-macro scale instability in 2D regular granular assemblies." *Continuum Mech. and Thermodynamics*, DOI 10.1007/s00161-013-0330-9

[86] Chang, C. S., and Yin, Z.-Y. (2011). "Micromechanical modeling for behavior of silty sand with influence of fine content." *Int. J. of Solids and Structures*, 48(19), 2655-2667.

[87] Chang, C. S., and Meidani, M. (2013). "Dominant grains network and behavior of sand-silt mixtures: stress-strain modeling," *Int. J. for Numerical and Anal. Methods in Geomechanics*, 37(15), 2563-2589.

[88] Yin, Z.-Y., Zhao, J., and Hicher, P.-Y. (2014). "A micromechanics-based model for sand-silt mixtures." *Int. J. of Solids and Structures*, 51(6), 1350-1363.

[89] Yin, Z.-Y., Chang, C. S., and Hicher, P.-Y. (2010). "Micromechanical modelling for effect of inherent anisotropy on cyclic behaviour of sand." *Int. J. of Solids and Structures*, 47(14-15), 1933-1951.

[90] Hicher, P. Y., Chang, C. S., and Dano, C. (2008). "A Multi-Scale Modeling of Grouted Sand." *Int. J. of Solids and Structures*, 45(16), 4362-4374.

[91] Misra, A., and Yang, Y. (2010). "Micromechanical model for cohesive materials based upon pseudo-granular structure." *Int. J. of Solids and Structures*, 47(21), 2970-2981.

[92] Hicher, P.Y. and Chang, C. S. (2007). A microstructural elastoplastic model for unsaturated granular materials", *Int. J. of Solids and Structures*, 44(7-8), 2304-2323.

[93] Chang, C. S., and Hicher, P. Y. (2009). "A model for granular materials with surface energy forces." *Int. J. of Aerospace Engrg.*, 22(1), 43-52.

[94] Hicher, P. Y. (2013). "Modelling the impact of particle removal on granular material behaviour." *Géotechnique*, 63(2), 118-128.

[95] Misra, A., and Singh, V. (2013). "Micromechanical model for viscoelastic-materials undergoing damage." *Continuum Mech. and Thermodynamics*, 25(2-4), 343-358.

[96] Misra, A., and Singh, V. (2014b). "Nonlinear granular micromechanics model for multi-axial rate-dependent behavior." *Int. J. of Solids and Structures*, 51(13), 2272-2282.

[97] Yang, Y., and Misra, A. (2012). "Micromechanics based second gradient continuum theory for shear band modeling in cohesive granular materials following damage elasticity." *Int. J. of Solids and Structures*, 49(18) 2500–2514.

[98] Souza, F. V., and Allen, D. H. (2011). "Modeling the transition of microcracks into macrocracks in heterogeneous viscoelastic media using a two-way coupled multiscale model." *Int. J. of Solids and Structures*, 48(22), 3160-3175.

[99] Greene, M. S., Li, Y., Chen, W., and Liu, W. K. (2013). "The archetype-genome exemplar in molecular dynamics and continuum mechanics." *Comput. Mech.*, 1-51.

[100] Nitka, M., Combe, G., Dascalu, C, and Desrues, J. (2011). "Two-scale modeling of granular materials: a DEM-FEM approach." *Granular Matter*, 13(3), 277–281.

[101] Zhao, J., and Guo, N. (2014). "Bridging the micro and macro for granular media: a computational multiscale paradigm." IS-Cambridge 2014: the Second Int. Symposium on Geomechanics from Micro to Macro. 1-3 September 2014, Cambridge, UK.

[102] Lim, K. W., and Andrade, J. E. (2013). "Granular Element Method (GEM) for three-dimensional discrete element calculations." *Int. J. for Numerical and Anal. Methods in Geomechanics*, 38(2), 167-188.

[103] Mollon, G., and Zhao, J. D. (2012). "Fourier-Voronoi-based generation of realistic samples for discrete modeling of granular materials." *Granular Matter*, 14(5), 621-638.

[104] Mollon, G, and Zhao, J. D. (2014). "3D generation of realistic granular samples based on random fields theory and Fourier shape descriptors." *Computer Methods in Appl. Mech. and Engrg.*, 279, 46-65.

[105] Potyondy, D. O., and Cundall, P. A. (2004). "A bonded-particle model for rock." *Int. J. of Rock Mech. & Mining Sciences*, 41(8), 1329-1364.

[106] Ferellec, J. F., and McDowell G. R. (2010). “A method to model realistic particle shape and inertia in DEM.” *Granular Matter*, 12(5), 459-467.

[107] Gao, R., Du, X., Zeng, Y., Li, Y., and Yan, J. (2012). “A new method to simulate irregular particles by discrete element method.” *J. of Rock Mech. and Geotechnical Engrg.*, 4(3), 276-281.

[108] Sun, S., and Shen, H. H. (2012). “Simulation of pancake ice load on a circular cylinder in a wave and current field.” *Cold Regions Science and Technol.*, 78, 31-39.

[109] Boton, M., Azema, E., Estrada, N., Radjai, F., and Lizcano, A. (2013). “Quasistatic rheology and microstructural description of sheared granular materials composed of platy particles.” *Phys. Rev. E*, 87(3), 032206.

[110] Galindo-Torres, S. A. (2013). “A coupled discrete element lattice Boltzmann method for the simulation of fluid-solid interaction with particles of general shapes.” *Computer Methods in Appl. Mech. and Engrg.*, 265, 107-119.

[111] Zhang, L., Quigley, S. V., and Chan A. H. C. (2013). “A fast scalable implementation of the two-dimensional triangular discrete element method on a GPU platform.” *Advances in Engrg. Software*, 60/61, 70-80.

[112] Zhou, W., Ma. G., Chang, X. L., Zhou, C. B. (2013). “Influence of particle shape on behavior of rockfill using a three-dimensional deformable DEM.” *J. Eng. Mech*., ASCE, 139(2), 1868-1873.

[113] Kuhn, M. R. (2011). “Implementation of the Jager contact model for discrete element simulations.” *Int. J. for Numerical Methods in Engrg.*, 88(1), 66-82.

[114] Cavarretta, I., Coop, M., and O’Sullivan, C. (2010). “The influence of particle characteristics on the behaviour of coarse grained soils.” *Geotechnique*, 60(6), 413-423.

[115] Cole, D. M., Mathisen, L. U., Hopkins, M. A., and Knapp, B. R. (2010). “Normal and sliding contact experiments on gneiss.” *Granular Matter*, 12(1), 69-86.

[116] Li, S. Q., Marshall, J. S., Liu, G. Q., and Yao, Q. (2011). “Adhesive particulate flow: The discrete-element method and its application in energy and environmental Engrg..” *Progress in Energy and Combustion Science*, 37, 633-668.

[117] Sümer,B., and Sitti M. (2008). “Rolling and spinning friction characterization of fine particles using lateral force microscopy based contact pushing.” *J. of Adhesion Science and Technol.*, 22(5-6), 481-506.

[118] Marshall, J. S., and Li, S. Q. (2014). *Adhesive particle flow: a discrete-element approach*, Cambridge University Press.

[119] Marshall, J. S. (2008). “Discrete-element modeling of particulate aerosol flows.” *J. of Comput. Physics*, 228, 1541-1561.

[120] Liu, G., Marshall, J. S., Li, S. Q., and Yao, Q. (2010). “Discrete-element method for particle capture by a body in an electrostatic field.” *Int. J. For Numerical Methods In Engrg.*, 84(13), 1589-1612.

[121] Wang, L., Park, J.-Y. and Fu, Y. (2007). “Representation of real particles for DEM simulation using X-ray tomography.” *Construction and Building Mater.*, 21(2), 338-346.

[122] Huang, H., and Tutumluer, E. (2014). “Image-aided element shape generation method in discrete-element modeling for railroad ballast.” *J. of Mater. in Civil Engrg.*, 26(3), 527-535.

[123] Yang, X., You, Z., Jin, C., and Wang, H. (2015). “Aggregate numerical representation construction Using a ball growth model based on realistic aggregate shapes.” Transportation Res. Board 94th Annual Meeting, 2015, Washington DC, Transportation Research Board.

[124] Latham, J.-P., Munjiza, A., Garcia, X., Xiang, J., and Guises, R. (2008). “Three-dimensional particle shape acquisition and use of shape library for DEM and FEM/DEM simulation.” *Minerals Engrg.*, 21(11), 797-805.

[125] Chung, Y. C., and Ooi J. Y. (2012). “Linking of discrete element modelling with finite element analysis for analyzing structures in contact with particulate solid.” *Powder Technol.*, 217, 107-120.

[126] Zang, M., Gao, W., and Lei, Z. (2011). “A contact algorithm for 3D discrete and finite element contact problems based on penalty function method.” *Comput. Mech.*, 48, 541-550.

[127] Tran, V. D. H., Meguid, M. A., and Chouinard, L. E. (2013). “A finite-discrete element framework for the 3D modeling of geogride soil interaction under pullout loading conditions.” *Geotextiles and Geomembranes*, 37, 1-9.

[128] Munjiza, A., Lei, Z., Divic, V., and Peros, B. (2013). "Fracture and fragmentation of thin shells using the combined finite-discrete element method." *Int. J. for Numerical Methods in Engrg.*, 95(6), 478-498.

[129] Longmore, J.-P., Marais, P., and Kuttell, M. M. (2013). "Towards realistic and interactive sand simulation: A GPU-based framework." *Powder Technol.*, 235, 983-1000.

[130] Feng, C., Li, S. H., Liu, X. Y., and Zhang, Y. A. (2014). "A semi-spring and semi-edge combined contact model in CDEM and its application to analysis of Jiweishan landslide." *J. of Rock Mech. and Geotechnical Engrg.*, 6, 26-35.

[131] Zhu, H. P., Zhou, Z. Y., Yang, R. Y., and Yu, A. B. (2008). "Discrete particle simulation of particulate systems: A review of major applications and findings." *Chemical Engrg. Science*, 63(13), 5728-5770.

[132] Liu, S. H., Sun, D. A., and Wang, Y. (2003). Numerical study of soil collapse behavior by discrete element modelling. *Computers and Geotechnics*, 30(5), 399-408.

[133] Yang, R. Y., Zou, R. P., and Yu, A. B. (2003). "Numerical study of the packing of wet coarse uniform spheres." *AIChE J.*, American Institute of Chemical Engineers, 49(7), 1656-1666.

[134] Tsuji, Y., Kawaguchi, T., and Tanaka, T. (1993). "Discrete particle simulation of two-dimensional fluidized bed. " *Powder Technol.*, 77, 79-87.

[135] El Shamy, U., and Aydin, F. (2008). "Multi-scale modeling of flood-induced piping in river levees." *J. of Geotechnical and Geoenvironmental Engrg.*, 134(9), 1385-1398.

[136] El Shamy, U., and Zeghal, M. (2007). "A micro-mechanical investigation of the dynamic response and liquefaction of saturated granular soils." *Soil Dynamics and Earthquake Engrg.*, 27(8), 712-729.

[137] Patankar, N. A., Huang, P. Y., and Ko, T., and Joseph, D.D. (2001). "Lift-off of a single particle in Newtonian and viscoelastic fluids by direct numerical simulation." *J. Fluid Mech.*, 438, 67-100.

[138] Zhu, Y., Fox, P., and Morris, J. (1999). "A pore-scale numerical model for flow through porous media." *Int. J. Numer. Anal. Methods Geomech.*, 23(9), 881-904.

[139] Potapov, A., Hunt, M., and Campbell, C. (2001). "Liquid–solid flows using smoothed particle hydrodynamics and the discrete element method." *Powder Technol.*, 116, 204-213.

[140] Cleary, P., Sinnott, M., and Morrison, R. (2006). "Prediction of slurry transport in SAG mills using SPH fluid flow in a dynamic DEM based porous media." *Miner. Engrg.*, 19, 1517-1527.

[141] El Shamy, U., and Abdelhamid, Y. (2014). "Modeling granular soils liquefaction using coupled lattice Boltzmann method and discrete element method." *Soil Dynamics and Earthquake Engrg.*, 67, 119-132.

[142] Abdelhamid, Y., and El Shamy, U. (2014). "Pore-scale modeling of surface erosion in a particle bed." *Int. J. for Numerical and Anal. Methods in Geomechanics*, 38(2), 142-166.

[143] Lomine, F., Scholts, L. ,Sibille, L., and Poullain, P. (2011). "Modeling of fluid solid interaction in granular media with coupled lattice Boltzmann/discrete element methods: Application to piping erosion." *Int. J. for Numerical Methods in Engrg.*, 37(6), 577-596.

[144] Ladd, A. J. C. (1994). " Numerical simulations of particulate suspensions via a discretized Boltzmann equation: Part 2. Numerical results." *J. of Fluid Mech.*, 271, 311-339.

[145] Wen, H., and Zhang, K. (2014). "Coupling discrete-element method and computation fluid mechanics to simulate aggregates heating in asphalt plants." *J. Engrg. Mech.*, 04014129.

[146] Tsang, C.F., Jing, L.R., Stephansson, O., and Kautsky, F. (2005). "The DECOVALEX III project: A summary of activities and lessons learned." *Int. J. of Rock Mech. and Mining Sciences*, 42(5-6), 593-610.

[147] Rutqvist, J., Backstrom, A., Chijimatsu, M., Feng, X. T., Pan, P. Z., Hudson, J., Jing, L., Kobayashi, A., Koyama, T., Lee, H. S., Huang, X. H., Rinne, M., and Shen, B. T. (2009a). "A multiple-code simulation study of the long-term EDZ evolution of geological nuclear waste repositories." *Environmental Geology*, 57(6), 1313-1324.

[148] Rutqvist, J., Vasco, D. W., and Myer, L. (2009b). "Coupled reservoir-geomechanical analysis of CO2 injection at In Salah, Algeria." *Energy Procedia*, 1, 1847-1854.

[149] Romagnoli, P., Arias, A., Barelli, A., Cei, M., and Casini, M. (2010). "An updated numerical model of the Larderello–Travale geothermal system, Italy." *Geothermics*, 39, 292-313.

[150] Itasca Consulting Group, I. (2014). Thermal Option, pp. Options and Add-ons.

[151] Tomac, I. (2014). "Micro-mechanical Aspects of Hydraulic Fracture Propagation and Proppant Flow and Transport for Stimulation of Enhanced Geothermal Systems: A Discrete Element Study." Colorado School of Mines.

[152] Min, K.-B., Rutqvist, J., and Elsworth, D. (2009). "Chemically and mechanically mediated influences on the transport and mechanical characteristics of rock fractures." *Int. J. of Rock Mech. and Mining Sciences*, 46(1), 80-89.

[153] Fauriel, S., and Laloui, L. (2012). "A bio-chemo-hydro-mechanical model for microbially induced calcite precipitation in soils." *Computers and Geotechnics*, 46, 104-120.

[154] Yasuhara, H., Elsworth, D., and Polak, A. (2003). "A mechanistic model for compaction of granular aggregates moderated by pressure solution." *J. Geophys. Res.-Sol. Ea.*, 108(B11), 2530.

[155] Zheng, B.S., and Elsworth, D. (2012). "Evolution of permeability in heterogeneous granular aggregates during chemical compaction: Granular mechanics models." *J. Geophys. Res.-Sol. Ea.*, 117(B3), B03206.

[156] Kumaran, V. (2005). "Kinetic model for sheared granular flows in the high Knudsen number limit." *Phys. Rev. Letters*, 95, 108001.

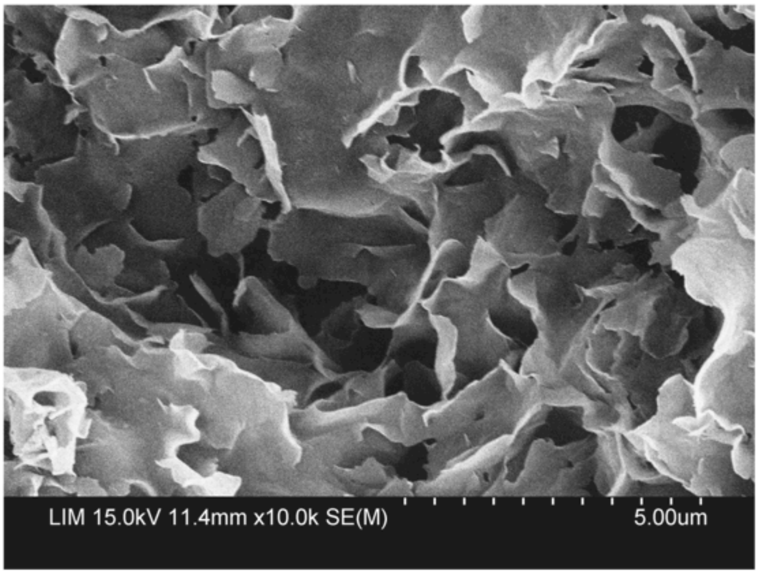

Figure 1. Smectite particles observed by SEM technique.

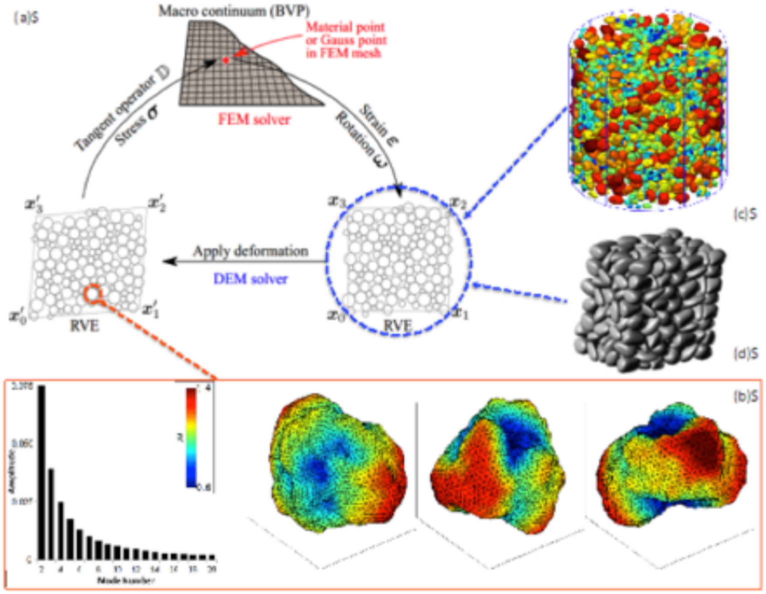

Figure. 2 Hierarchical multiscale modeling (HMM) for granular media accounting for realistic particle morphology (a) Schematic of the HMM method [75]; (b) Modeling 3D shape of granular particles based on Fourier shape descriptor and Random field theory [104]; (c) Packing of generated complex shaped particles into a cylindrical container as RVE [104]; (d) Assembly of complex shape particles based on NURBS technique as RVE [102].