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Micro origins for macro behavior in granular media

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Abstract We report the latest advances in understanding, characterization and modeling of key micro mechanisms and origins underpinning the interesting and complex macroscopic behavior of granular matter. Included in this Topical Collection are novel theories, innovative experimental tools and new numerical approaches, focusing primarily on three subtopics governing important multiscale properties of granular media: (a) the jamming transition from fluid- to solid-like behavior, critical state flow and wave propagation, (b) the signature of fabric and its evolution for granular media under general loading conditions, and (c) mechanisms like rotation, breakage, failure and aggregation. The significance of these contributions and exploratory future directions pertaining to cross-scale understanding of granular matter are discussed.

Keywords Granular matter · Micro–macro transition · Multiscale modeling · Jamming transition · Granular flow · Fabric evolution · Particle breakage · Failure · Clay aggregation

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1 Introduction

Granular media are amongst the most widespread materials on the earth and are of tremendous importance to a great variety of engineering and industrial branches, including civil and chemical engineering, pharmaceutical and mining industries. The poorly understood behavior of granular media has long been claimed to be mysterious and complicated. Under both confined or unconfined loads, they exhibit exceedingly complex responses such as strong nonlinearity, loading path dependency, stress dilatancy, anisotropy, non-coaxiality, critical state flow, grain breakage, liquefaction, failure and jamming transition. Hinged to these complicated macroscopic observations on granular media are key underlying mechanisms and origins on the much more detailed microscopic level; as stated: "*To see a world in a grain of sand*" by William Blake. Information identifiable from the grain-scale can greatly help to reveal the rich world of granular media. Indeed, there has been collective effort made by the community of granular mechanics and granular physics towards systematic examination and characterization of the multiscale nature of granular media for an improved understanding of their behavior. This topical collection reports on the latest progresses in this line of research. It includes a total of ten contributions from prominent researchers working in this area, nine of which based on substantial extensions of their works presented in the Second International Symposium on "Geomechanics from Micro to Macro" held at Cambridge University from September, 1–4, 2014. The topical collection covers three major topics and their inter-relation: (1) the jamming transition from fluid to solid, flow and wave propagation in solids; (2) signatures of the microstructure (fabric) and fabric evolution, as well as (3) breakage, failure and aggregation in granular media.

2 Jamming, flow and waves

The transition between jammed (solid-like) and unjammed (fluid-like) states in granular media has been a research topic of both theoretical importance and practical significance [1–4]. Of fundamental importance for understanding the behavior of a granular material is the jamming density (above which the material exhibits stable mechanical response but becomes unstable if below). There have been persistent debates over the existing of a unique jamming density for a granular material signifying the occurrence of a jamming transition, resembling the critical phenomena. Recent theoretical and experimental studies indicate that the jamming density may depend crucially on the preparation protocol and is a loading history sensitive state-variable [2]; consequently, the jamming transition may occur over a considerable range of densities [5–7]. A unified theoretical model that can provide reconciling explanations over various contradictory observations on jamming transitions is highly desirable but unavailable so far. Kumar and Luding [8] made a significant step forward in this direction. They proposed a simple, working model for the jamming transition and its history dependence, based on particle-scale observations, by incorporating the jamming density as a state variable, to link the macroscopic behavior of granular systems to their underpinning microstructures. Their framework involves an effective multiscale model of jamming and un-jamming under different loading conditions, where isotropic compression and shearing lead to qualitatively different response of the systems microstructure and thus the jamming density. Unified, quantitative explanations were offered, based on the frictionless model system predictions, for varied flow patterns. This line of research may provide important insights for key engineering applications in geoscience, geology and industrial processes.

A typical unjammed state of granular media is the case of unconfined granular flow, e.g. down an incline. In geotechnical engineering, it may be present in specific forms such as gravity-driven debris flow that is frequently too complicated to be characterized by existing granular flow theories. Debris flow typically consists of particles of sizes ranging over six orders of magnitude. Furthermore, being a mixture of particles and fluid, debris flow may exhibit highly inhomogeneous compositions from its front to tail due to grain size segregation, channel bed entrainment and other processes [9,10]. Due to its highly polydisperse nature in particle size with often irregular features in particle shape, one particular challenge towards understanding the stress transfer mechanics in dense debris flow is the accurate measurement of the random particle velocity fluctuations, or so-called "granular temperature", related to the collisional stress transfers among different particle groups. Using flume tests of debris flow consisting of a mixture of graded glass particles and a refractively matched fluid, Sanvitale and Bowman [11] examined the capacity and limitations of Particle Image Velocimetry (PIV) on measuring the fluctuating velocity field in the interior of polydisperse, unsteady and segregating flows, and provided useful observations towards an improved understanding of debris flow.

Another important issue in geotechnical engineering is to assess the serviceability of geo-structures (such as foundations and embankments) pertaining to granular soils, which require accurate measurements of the small-strain stiffness of the soil. Commonly used dynamic testing approaches include those based on resonant column tests and the measurement of body wave velocities within a soil element test. Related to such tests, a particular challenge lies in the interpretation of the measured data, which demands advanced knowledge on wave propagation theory in the framework of continuum mechanics [12]. O'Donovan et al. [13] developed a multi-axial testing apparatus installed with point source transmitters and receivers to evaluate the shear and compression wave velocities of samples. They compared their experimental data on seismic wave propagation in granular media by this apparatus with both DEM simulations and continuum modeling results. The DEM results extracted from the particle-scale of their simulations facilitated a detailed frequency domain analysis of energy dissipation during wave propagation in a granular sample, and corroborated a better interpretation of the dynamic testing data leading towards improved continuum theory models.

3 Signatures of fabric and fabric evolution

A rather perplexing aspect of granular materials is the strong dependence of their responses on loading conditions and/or stress paths. Under different loading conditions, the same material may behave entirely differently. This has led to numerous unanswered questions for constitutive modeling. Considerable efforts have been made by the community attempting to develop universal models capable of predicting the behavior of granular under varying loading conditions. However, the prevailing purely phenomenological approaches have largely failed to attain this goal. Active attempts have recently been diverted to identify the key microstructures and micromechanisms that act as difference makers for the varied macroscopic responses under different loading conditions to be used in modern constitutive modeling [8,14–23]. The signature of the microstructure of granular media under cyclic loads has been and still is an issue of particular interest.

In their DEM simulations, Wang and Wei [24] defined a particle-void fabric which they called average "centroid distance", D_c, to quantify the microstructural changes in a granular assembly during undrained cyclic loading, especially during cyclic mobility and post-liquefaction stage. Their micromechanical results indicate that strong correlations exist between D_c, the cyclic mobility and the post-liquefaction deformation. A low value of D_c implies a stable state of particle-void distributions achievable in post liquefaction, whilst a highly anisotropic angular distribution of D_c, found during the post-liquefaction stage, implies a highly anisotropic internal structure providing higher load bearing capacity for an assembly.

Jiang et al. [25] investigated the evolution of fabric within a DEM assembly consisting of elliptical particles under both monotonic and cyclic constant volume simple shear tests. They found in both shearing conditions that the particle-orientation-based fabric was much harder to be mobilized to evolve than the contact normal or force based fabric, which confirms the observations by Zhao and Guo [26,27] in earlier multiscale studies on the interplay between fabric anisotropy and strain localization. Rotational cyclic loading has been a typical non-proportional test, widely encountered in soils during earthquake and offshore/coastal wave loads, and has been proven difficult to model within a continuum mechanical framework. Li et al. [28] carried out 3D DEM simulations to examine the relation between deformation and fabric structure for a dense assembly subjected to a continuous rotation of the (applied) principal stress direction. Using the contact-based fabric tensor, they found that the rotation of the principle stress axes led to densification of their samples with greater coordination numbers and cyclically varying fabric anisotropy, as also reported by Kumar et al. [17].

Internal erosion of gap-graded soils can cause instability of the soil structure and pose great safety threats to dams or flood embankments [29] and coarse-fine particle ratio can be an important index affecting the erodability of gap-graded soils [30]. Based on DEM simulations of a bimodal assembly as a simple gap-graded soil, Shire et al. [31] examined the particle-scale fabric information related to the interplay between fine and coarse particles in the assembly under isotropic compression. They identified key size ratios and fines contents, when the transitions of the soil fabric occur, to be closely correlated to microscopic changes governing the contact distributions and stress-transfer characteristics of the soils as well as the size (distribution) of the void space between coarse particles.

4 Rotation, breakage, failure and aggregation

In particulate soils, the constituent particles may slide, rotate and break and can result in failure of an assembly in form of either localized or diffuse failure patterns [32–34]. The particles may also aggregate to form structures affecting the overall behavior of soil. Particle crushing is of great interest to multiple disciplines including mineral and mining engineering, powder technology, geology and geophysics [35]. Through its influence on the grain and pore size distributions, particle breakage has long been identified as a key micromechanism governing the macroscopic behavior of granular media [36]. Grain shape is among the key factors influencing the crushability of a sand grain, and clumped particles have been widely used in DEM simulations of particle crushing to account for the shape effect [37]. Using two-ball clumps in their DEM modeling, de Bono and McDowell [38] investigated the effects of particle shape on the normal compression and subsequent over-consolidation of a crushable soil sample. They demonstrated that the slope of the normal compression line depends solely on the particle size-hardening law according to a linear relationship in log-log plots. Furthermore, the use of clumped particles offers more realistic predictions of the coefficient of lateral earth pressure. Simulations of particle crushing based on even more realistic grain shapes will thus continue to be a research topic of broad interest.

The complex failure patterns exhibited by granular media, including localized, diffuse and divergent modes, have attracted sustained interest in the community of both geomechanics and geophysics. Traditionally, many relevant studies have been carried out based on experiments or continuum modeling [39,40]. The trend in methodology on this topic has recently shifted to combined, multiple approaches including advanced experimental tools such as X-Ray CT [41] and discrete element methods or computational multiscale modeling approaches [26,42]. Hadda et al. [43] employed the discrete element method to examine particle-level energy decomposition in relation with their signature contributions to macroscopic failure modes including shear banding and diffuse failure. In particular, they followed an energy-based approach by decomposing the external energy into elastic, plastic and kinetic parts and extracted each contributing portion from their DEM simulations to establish correlations with the macroscopic failure modes for a given sample. As a main result, they found interesting similarities between shear band and diffuse mode failure in terms of their energy signatures.

Particulate systems can be very different: whilst sand particles might break, other particles will aggregate. Clay particles, for example, interact by electrostatic and van der Waals forces. Their aggregation may cause significant changes of the microstructure but also of their macro-mechanical behavior of clays. It has been tremendously challenging to characterize the stability of clay-water systems at short-range length-scales where clay aggregates are formed. Based on molecular dynamics (MD) simulations of interactions between two layers of Wyoming montmorillonite (Na-smectite) in bulk water, Ebrahimi et al. [44] established correlations between clay aggregate formation and the mechanical properties related to clay platelet layer interactions, leading to improve the understanding of meso-scale aggregation of clay platelets in water. This helps to identify some of the key molecular-scale origins for the many complicated macroscopic behaviors of clay as an example of realistic, complex multi-physics and multiscale granular matter.

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References

1. Bi, D., Zhang, J., Chakraborty, B., Behringer, R.P.: Jamming by shear. Nature **480**, 355–358 (2011)
2. Luding, S.: Granular matter: so much for the jamming point. Nat. Phys. **12**, 531–532 (2016). doi:10.1038/nphys3680
3. Yu, A., Dong, K., Yang, R., Luding, S.: Powders and Grains 2013. In: AIP Conference Proceedings #1542. American Institute of Physics (2013). ISBN 978-0-7354-1166-1
4. Nakagawa, M., Luding, S.: Powders and Grains 2009. In: AIP Conference Proceedings #1145. American Institute of Physics (2009). ISBN 978-0-7354-0682-7
5. Liu, A.J., Nagel, S.R.: The jamming transition and the marginally jammed solid. Annu. Rev. Condens. Matter Phys. **1**, 347–369 (2010)
6. Torquato, S., Stillinger, F.H.: Jammed hard-particle packings: from Kepler to Bernal and beyond. Rev. Mod. Phys. **82**, 26–33 (2010)
7. Majmudar, T.S., Sperl, M., Luding, S., Behringer, R.P.: Jamming transition in granular systems. Phys. Rev. Lett. **98**, 058001 (2007)
8. Kumar, N., Luding, S.: Memory of jamming—multiscale flow in soft and granular matter. Granular Matter (2016). doi:10.1007/s10035-016-0624-2
9. Johnson, C.G., Kokelaar, B.P., Iverson, R.M., Logan, M., LaHusen, R.G., Gray, J.M.N.T.: Grain size segregation and levee formation in geophysical mass flows. J. Geophys. Res. **117**, F01032 (2012). doi:10.1029/2011JF002185
10. Mutabaruka, P., Delenne, J.-Y., Soga, K., Radjai, R.: Initiation of immersed granular avalanches. Phys. Rev. E **89**(5), 052203 (2014)
11. Sanvitale, N., Bowman, E.T.: Using PIV to measure granular temperature in saturated unsteady polydisperse granular flow. Granular Matter (2016). doi:10.1007/s10035-016-0620-6
12. Mutabaruka, P., Kumar, K., Soga, K., Radjai, F., Delenne, J.-Y.: Transient dynamics of a 2D granular pile. Eur. Phys. J. E **38**, 47 (2015)
13. O'Donovan, J., Ibraim, E., O'Sullivan, C., Hamlin, S., Muir Wood, S.D., Marketos, G.: Micromechanics of seismic wave propagation in granular materials. Granular Matter (2016). doi:10.1007/s10035-015-0599-4
14. Guo, N., Zhao, J.D.: The signature of shear-induced anisotropy in granular media. Comput. Geotech. **47**, 1–15 (2013). doi:10.1016/j.compgeo.2012.07.002
15. Yimsiri, S., Soga, K.: DEM analysis of soil fabric effects on behaviour of sand. Géotechnique **60**(6), 483–495 (2010)
16. Yimsiri, S., Soga, K.: Effects of soil fabric on behaviors of granular soils: microscopic modeling. Comput. Geotech. **38**(7), 861–874 (2011)
17. Kumar, N., Luding, S., Magnanimo, V.: Macroscopic model with anisotropy based on micro-macro information. Acta Mech. **225**, 2319–2343 (2014)
18. Jiang, M.J., Zhang, F.G., Sun, Y.G.: An evaluation on the degradation evolutions in three constitutive models for bonded geomaterials by DEM analyses. Comput. Geotech. **57**, 1–16 (2014)
19. Jiang, M.J., Zhu, H.H.: An interpretation of the internal length in Chang's couple-stress continuum for bounded granulates. Granular Matter **9**, 431–437 (2007)
20. Jiang, M.J., Harris, D., Zhu, H.H.: Future continuum models for granular materials in penetration analyses. Granular Matter **9**, 97–108 (2007)
21. Jiang, M.J., Yu, H.S., Harris, D.: Kinematic variables bridging discrete and continuum granular mechanics. Mech. Res. Commun. **33**, 651–666 (2006)
22. Jiang, M.J., Harris, D., Yu, H.S.: Kinematic models for non-coaxial granular materials: Part I: Theories. Int. J. Numer. Numer. Methods Geomech. **29**(7), 643–661 (2005)
23. Jiang, M.J., Harris, D., Yu, H.S.: Kinematic models for non-coaxial granular materials: Part II: Evaluation. Int. J. Numer. Numer. Methods Geomech. **29**(7), 663–689 (2005)
24. Wang, G., Wei, J.T.: Microstructure evolution of granular soils in cyclic mobility and post-liquefaction process. Granular Matter (2016). doi:10.1007/s10035-016-0621-5
25. Jiang, M.J., Li, T., Shen, Z.F.: Fabric rates of elliptical particle assembly in monotonic and cyclic shear tests: a numerical study. Granular Matter (2016). doi:10.1007/s10035-016-0641-1
26. Guo, N., Zhao, J.D.: A coupled FEM/DEM approach for hierarchical multiscale modelling of granular media. Int. J. Numer. Numer. Methods Geomech. **99**(11), 789–818 (2014)
27. Zhao, J.D., Guo, N.: The interplay between anisotropy and strain localization in granular soils: a multiscale insight. Géotechnique **65**(8), 642–656 (2015)
28. Li, X., Yang, D.S., Yu, H.S.: Macro deformation and micro structure of 3D granular assemblies subjected to rotation of principal stress axes. Granular Matter (2016). doi:10.1007/s10035-016-0632-2
29. Li, M., Fannin, R.J.: A theoretical envelope for internal instability of cohesionless soil. Géotechnique **62**, 449–460 (2011)
30. Yin, Z.Y., Zhao, J.D., Hicher, P.Y.: A micromechanics-based model for sand-silt mixtures. Int. J. Solids Struct. **51**(6), 1350–1363 (2014)
31. Shire, T., O'Sullivan, C., Hanley, K.J.: The influence of fines content and size-ratio on the micro-scale properties of dense bimodal material. Granular Matter (2016). doi:10.1007/s10035-016-0654-9
32. Herrmann, H.J.: Rotations in shear bands. In: Wall, W.A., Bletzinger, K.U., Schweizerhof, K. (eds.) Trends in Computational Structural Mechanics, pp. 140–144. CIMNE, Barcelona (2001)
33. Herrmann, H.J., Hovi, J.-P., Luding, S.: Physics of Dry Granular Media, vol. 350. Springer, Berlin (1998)
34. Jiang, M.J, Zhu, H.H., Harris, D.: Classical and non-classical kinematic fields of two-dimensional penetration tests on granular ground by discrete element method analyses. Granular Matter **10**, 439–455 (2008)
35. Einav, I.: Breakage mechanics. Part I: Theory. J. Mech. Phys. Solids **55**(6), 1274–1297 (2007). doi:10.1016/j.jmps.2006.11.003
36. Marketos, G., Bolton, M.D.: Quantifying the extent of crushing in granular materials: a probability-based predictive method. J. Mech. Phys. Solids **55**(10), 2142–2156 (2007). doi:10.1016/j.jmps.2007.03.003
37. Cheng, Y.P., Bolton, M.D., Nakata, Y.: Crushing and plastic deformation of soils simulated using DEM. Géotechnique **54**(2), 131–141 (2004). doi:10.1680/geot.2004.54.2.131
38. de Bono, J.P., McDowell, G.: Investigating the effects of particle shape on normal compression and overconsolidation using DEM. Granular Matter (2016). doi:10.1007/s10035-016-0605-5
39. Desrues, J., Viggiani, G.: Strain localization in sand: an overview of the experimental results obtained in Grenoble using stereopho-

togrammetry. Int. J. Numer. Anal. Methods Geomech. **28**(4), 279–321 (2004)
40. Gao, Z.W., Zhao, J.D.: Strain localization and fabric evolution in sand. Int. J Solids Struct. **50**, 3634–3648 (2013)
41. Ando, E., Hall, S.A., Viggiani, G., Desrues, J., Besuelle, P.: Grain-scale experimental investigation of localized deformation in sand: a discrete particle tracking approach. Acta Geotech. **7**(1), 1–13 (2012)
42. Andrade, J.E., Avila, C.F., Hall, S.A., Lenoir, N., Viggiani, G.: Multiscale modeling and characterization of granular matter: from grain kinematics to continuum mechanics. J. Mech. Phys. Solids **59**(2), 237–250 (2011)
43. Hadda, N., Sibille, L., Nicot, F., Wan, R., Darve, F.: Failure in granular media from an energy viewpoint. Granular Matter (2016). doi:10.1007/s10035-016-0639-8
44. Ebrahimi, D., Pellenq, R.J.M., Whittle, A.J.: Mesoscale simulation of clay aggregate formation and mechanical properties. Granular Matter (2016). doi:10.1007/s10035-016-0655-8