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A lattice discrete particle model for pressure-dependent inelasticity in granular rocks

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ABSTRACT

This paper details the formulation, calibration, and validation of a Lattice Discrete Particle Model (LDPM) for the simulation of the pressure-dependent inelastic response of granular rocks. LDPM is formulated in the framework of discrete mechanics and it simulates the heterogeneous deformation of cemented granular systems by means of discrete compatibility/equilibrium equations defined at the grain scale. A numerical strategy is proposed to generate a realistic microstructure based on the actual grain size distribution of a sandstone and the capabilities of the method are illustrated with reference to the particular case of Bleurswiller sandstone, i.e. a granular rock that has been extensively studied at the laboratory scale. LDPM micromechanical parameters are calibrated based on evidences from triaxial experiments, such as hydrostatic compression, brittle failure at low confinement and plastic behavior at high confinement. The results show that LDPM allows exploring the effect of fine-scale heterogeneity on the inelastic response of rock cores, achieving excellent quantitative performance across a wide range of stress conditions. In addition, LDPM simulations demonstrate its capability of capturing different modes of strain localization within a unified mechanical framework, which makes this approach applicable for a wide variety of geomechanical settings. Such promising performance suggests that LDPM may constitute a viable alternative to existing discrete numerical methods for granular rocks, as well as a versatile tool for the interpretation of their complex deformation/failure patterns and for the development of continuum models capturing the effect of micro-scale heterogeneity.

1. Introduction

Granular rocks display complex mechanical properties, such as the transition from brittle to ductile response upon increasing confinement,[1] the tendency to dilate or contract upon shearing,[2,3] and the formation of a wide range of strain localization mechanisms.[4–6] Such rich variety of deformation modes depends on the inelastic properties of rocks, and it is invariably controlled by the confining pressure. For example, while localized dilatant faulting is typically observed at low confinements, delocalized shear-enhanced compaction often characterizes the deformation response at high pressures. The transition from one type of response to another is typically gradual[1] and poses considerable challenges due to the competition of the microscopic processes that characterize each of the two aforementioned macroscopic phenomena. This intermediate behavior has been found to be crucial for a variety of applications, including the tectonics of faulting,[7–9] the coupling between strain localization and fluid flow,[10,11] reservoir compaction[12,13] and borehole instability.[14,15]

In the brittle faulting regime, the onset of dilatancy is associated with the propagation of cracks that align along directions subparallel to the maximum compressive stress. The coalescence of these cracks, as well as the frictional interaction between fractured and unfractured zones, ultimately leads to the onset of persistent shear bands, as well as to changes in physical properties, such as stiffness, permeability, and electrical conductivity.[16,17] In the cataclastic flow regime, grain crushing and pore collapse dominates the deformation process, ultimately leading to extensive densification of the rock mass. In high-porosity rocks, such micro-mechanical processes have been found to promote compaction bands, i.e. modes of strain localization characterized by the accumulation of compressive strains into narrow zones.[18,19] While these compaction localization processes are induced by a local loss of strength, the rearrangement of crushed fragments and the reduction of the local porosity often lead to a gradual transition to a delocalized mode of deformation.[20] As a result, unlike single shear bands, multiple compaction zones may propagate across the sample until a complete re-hardening of the specimen is observed.[21]

The prevalence of a specific form of microscopic damage depends on the microstructural attributes of a rock (e.g., grain size and sorting

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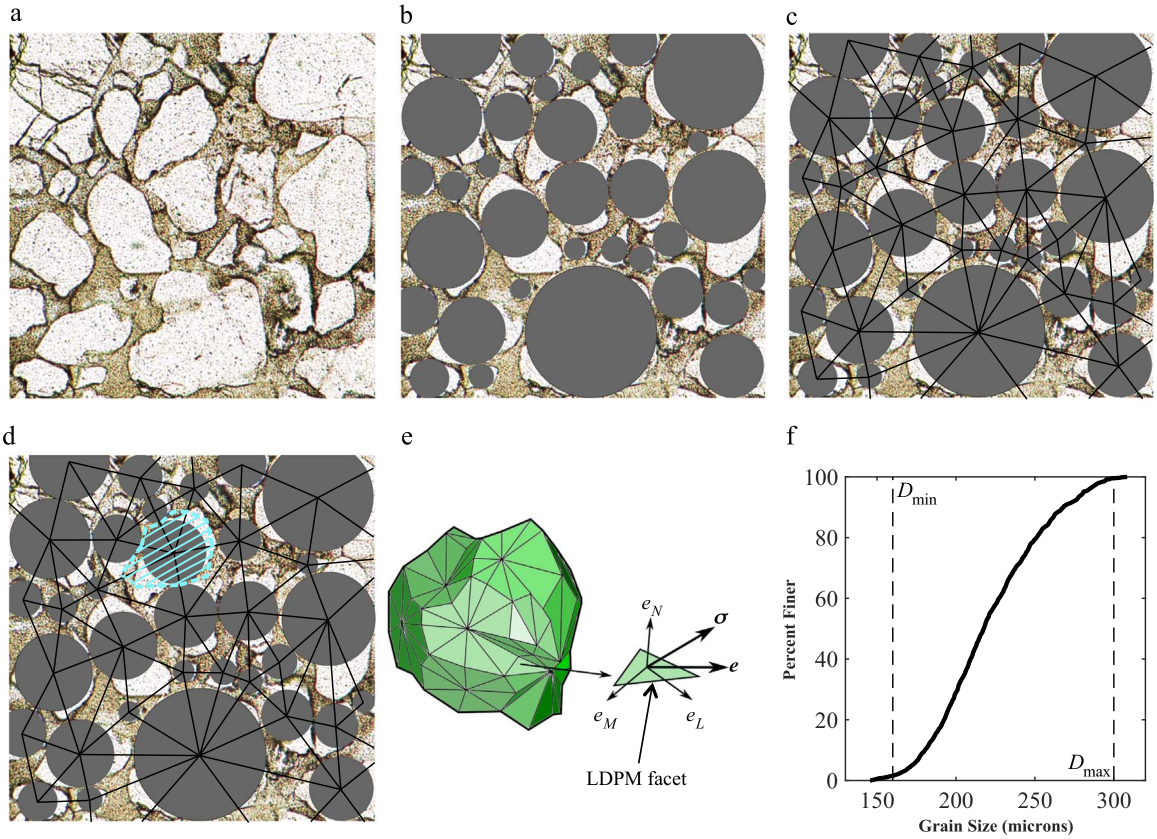

Fig. 1. (a) Microstructure of a sandstone. (b) Artificial supporting system for grain generation. (c) 2D representation of Delaunay tetrahedralization for the supporting system. (d) 2D representation of a polyhedral cell. (e) A 3D polyhedral cell/a LDPM cement-coated grain. (f) Grain size distribution of Bleurswiller sandstone used for the LDPM simulations.

porosity; degree of cementation), as well as by its inherent heterogeneity. Discrete mechanical methods are therefore convenient tools to accommodate grain-scale attributes and explain their impact on the macroscopic deformation of rock cores. For example, the discrete element method (DEM) has proved to be an effective tool for simulating the micromechanics of unconsolidated materials, such as soil, sediment and fault gouge.[22–25] DEM represents the material as an assemblage of independent particles interacting through forces computed on the basis of frictional contact models. Such methods have often been adapted to the case of lithified geomaterials by incorporating inter-particle bonds accounting for the presence of cementation, thus mimicking the nucleation of cracks though the brittle failure of cohesive cement bridges.[26,27] Such enhancements have enabled DEM to simulate complex processes such as the development of shear bands and brittle fracturing.[28,29]

Nevertheless, standard DEM techniques based on spherical particles tend to produce unrealistic ratios of uniaxial compressive to tensile strength,[30] thus hampering the satisfactory prediction of the failure characteristics of granular rocks deformed in the brittle faulting regime. Although this problem can be mitigated by increasing the density of bonds between particles[29,31] or by magnifying the grain interlocking through irregularly shaped particles,[32,33] the ability to capture the full spectrum of tensile and/or compressive failure mechanisms through a unified framework still represents a major challenge. Similar limitations exist also for simulations in the high-pressure regime, where DEM analyses are often used in conjunction with computationally intensive particle replacement schemes mimicking the effect of grain crushing.[34] While these approaches have provided insights into the interpretation of compaction localization, they often involve an unrealistic loss of grain mass, thus preventing a realistic simulation of crushing-induced hardening upon hydrostatic compression.[1]

To tackle these problems, this paper proposes an alternative discrete method that, by relying on a direct representation of the microstructure, aims to accommodate a wide range of inelastic mechanisms i.e., it enables accounting simultaneously for brittle/dilative modes of failure, as well as for the plastic regime of compactive deformation. The proposed approach builds upon the so-called Lattice Discrete Particle Model (LDPM), successfully developed by Cusatis and coworkers[35,36] for the simulation of failure processes in quasi-brittle solids such as concrete. A noticeable feature of LDPM is its ability to simulate a granular microstructure by means of a system of polyhedral particles connected through a three-dimensional lattice. Such particles can be placed randomly across the volume in accordance with a prescribed grain size distribution, thus enabling the direct representation of a heterogeneous system of grains surrounded by a bonding agent (e.g., mortar in concrete or mineral precipitants in natural rocks). At variance with DEM techniques, the kinematics of the skeleton is modeled on the basis of the displacements and rotations computed at the ends of the lattice connections, thus enabling the computation of strain components oriented normally and/or tangentially to the facets between the polyhedral particles. Such hypotheses imply the use of an internal kinematics substantially different from that of DEM. This facilitates the use of more sophisticated constitutive laws to model the forces transferred among adjacent particles. Recent works have demonstrated the ability of this approach to reproduce various aspects of quasi-brittle behavior, such as fracture initiation and propagation, shear banding, and frictional processes.[37–40] Therefore, LDPM offers a convenient platform to simulate the mechanics of sandstones, a particular class of quasi-brittle solids for which the pressure-dependent inelastic properties are primarily controlled by the heterogeneity of their grain skeleton. Although the strategy discussed hereinafter is in principle applicable to the analysis of any type of granular rock, here its capabilities are discussed for the particular case of Bleurswiller