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Research Paper

Numerical simulation of microstructure of brittle rock using a grain-breakable distinct element grain-based model

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ABSTRACT

A distinct element grain-based method (GBM) was developed to simulate the microstructure of rock-like materials. Using this method, a UDEC-GBM model can be readily constructed with a given mineral composition, allowing independent assignment of specific properties to both the grains and grain boundaries. Both intra-granular cracks cutting through the grains and inter-granular cracks developed along grain boundaries can be captured. These features allow a full incorporation of both geometric and mechanical heterogeneity at grain scale for simulating brittle rocks. The validity of the proposed UDEC-GBM approach was verified by simulating a low-porosity sandstone under compression and direct-shear tests. The UDEC-GBM was proved to be capable of reproducing many of the characteristics associated with brittle fracture in low-porosity sandstone. It was found that the model with unbreakable grains trends to under-estimate the crick initiation threshold, highlighting the importance of the incorporation of breakable grains when modeling micro-structure of brittle rocks. The numerical experiments suggested that examining the extent of the tensile stress zones alone may lead to a biased evaluation of tensile cracking at crack initiation. The tensile stress magnitude must also be taken into consideration. It was also found that a synthetic sandstone sample with relatively low ground boundary strength produces a more ductile post-peak behavior. Microscopic tensile strength of the grains has limited influence on the failure mechanism of the synthetic specimen under unconfined compression loading. The proposed GBM approach provides a very useful tool for studying grain-scale micro-mechanics of brittle rocks.

1. Introduction

Grain-scale microstructure controls the micromechanical behavior and hence the complex macroscopic response of intact rock. At the grain scale, a rock is composed of different materials (i.e., mineral, cements) and microstructural defects (i.e., microcracks) which promote microstructural heterogeneity. Microstructural heterogeneities can be due to geometric heterogeneity caused by the varying size and shape of grains, elastic heterogeneity due to varying stiffness of different grains, and contact heterogeneity resulting from anisotropy in contact distribution (length and orientation) and stiffness anisotropy [1]. It is widely accepted that heterogeneity plays a key role in the generation of localized tensile stresses resulting in crack initiation. However, our understanding of how heterogeneities affect the brittle rock failure mechanisms remains incomplete [2].

Due to significant developments in computer power over the last three decades, numerical modeling has become increasingly useful in simulating the mechanical behavior of rock materials. A common way of incorporating heterogeneity into numerical models is through the stochastic distribution of properties (e.g. Weibull distribution) [3,4]. This approach allows consideration of the elastic component of heterogeneities; however, incorporating geometric and contact heterogeneity requires a more sophisticated model in which grain structure (shape and size) can be realistically represented. In the literature, four methods are typically used to simulate grain structure: (1) disk-shaped grains [5,6] using the particle flow code PFC [7], (2) square-shaped grains using the code RFPA2D [8], (3) triangular grains [9,10] using the distinct element code UDEC [11] and hybrid finite-discrete codes Y-Geo [12] and ELFEN [13], (4) polygonal grains in UDEC [14,15]. The polygonal grain structure appears to be a more realistic representation of the microstructure of rock material. Conventional polygonal structure is usually generated in UDEC using the Voronoi tessellation technique. The Voronoi

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generator, however, generates a relatively uniform distribution of grain size. To solve this problem, Potyondy [16] developed the Grain Based Model (GBM) in which a rock is represented by a polygonal grain structure. The GBM allows users to incorporate different minerals with varying grain sizes. The implementation of the GBM has been included in both PFC and UDEC. In PFC, a polygonal grain is breakable as it is represented by an assembly of particles. PFC-GBMs have been used to simulate laboratory specimens subjected to compression [16–18], direct tension [16], and direct shear [18,19]. An intrinsic issue with the PFC-GBM approach when simulating low-porosity rock (<2%) is that a minimum porosity of 9% has to be incorporated in the model due to the circular shape of the particles. In Y-Geo, polyhedral grains can be incorporated by decomposing a grain into several elements, both inter-granular and intra-granular cracking are thus can be explicitly simulated [20,21]. Mahabadi et al. [20] used Y-Geo to simulate a crystalline rock of which the specific microstructure was incorporated in their models. In UDEC, a polygonal grain can be either deformable or rigid. UDEC-GBMs with unbreakable grains have been used to simulate laboratory specimens subjected to compressive loading [1,22]. As discussed in [2], a more representative simulation of microstructure and microstructural interaction would require breakable grains as grain boundary and mineral grain strengths are likely to provide different contributions to micromechanical behavior and hence macroscopic response.

In this study, the authors propose a novel grain-breakable UDEC-GBM model to simulate low-porosity rock material. This method allows a more sophisticated representation of microstructure with deformable, breakable polygonal grains cemented along their adjoining sides. The proposed approach is capable of incorporating different types of minerals for which different stiffness and strength properties can be considered. Both intra-granular cracking inside minerals and inter-granular cracking developed along grain boundaries can be simulated. These features help to improve our understanding of microstructural failure mechanisms and hence macroscopic failure mechanisms of low-porosity sandstone.

2. The grain-breakable UDEC-GBM model

The proposed UDEC-GBM model initially uses the PFC code to generate a polygonal grain structure using a two-dimensional disk-packing scheme based on the following procedure [16]: (1) create a bonded particle model that has no walls and in which each particle must have at least two contacts; the types of desired grains and their size can be controlled by the particle size, Fig. 1a; (2) identify the void centroids between particles, Fig. 1b; and (3) generate a polygonal network by joining the centroids with lines, Fig. 1c and d. The generated grain structure, described by a 2D mesh consisting of nodes, edges and elements, is then exported from PFC and imported into UDEC.

In UDEC, the imported grains are represented as intact blocks and can be either rigid or deformable. The contacts joining two opposing blocks are regarded as inter-granular bonds representing the cement. To make the grains breakable, each grain is discretized into several triangular blocks by creating several contacts from the center of the grain to its apex, Fig. 1e. These contacts are defined as intra-granular bonds, distinguishing them from inter-granular. The intra-granular bonds provide potential paths along which a crack can pass through the grain. An Intra-granular crack occurs when an intra-granular bond breaks; in contrast, a inter-granular crack occurs due to breakage of a inter-granular bond along a grain boundary. Further discretization may also be performed to cut each triangular block into three sub-triangular blocks, Fig. 1f. Although a denser discretization increases the potential number of paths for intra-granular cracking, this in turn increases the number of blocks and contacts threefold, leading to a significant increase in demand in terms of computer runtime. It should also be noted the second order mesh refinement inside grains leads to poor element geometry and an optimized meshing algorithm is required for further investigation.

The mechanical behavior of the contacts (representing both intra- and inter bonds) is controlled by the Coulomb friction law. In the direction normal to a contact, the stress-displacement

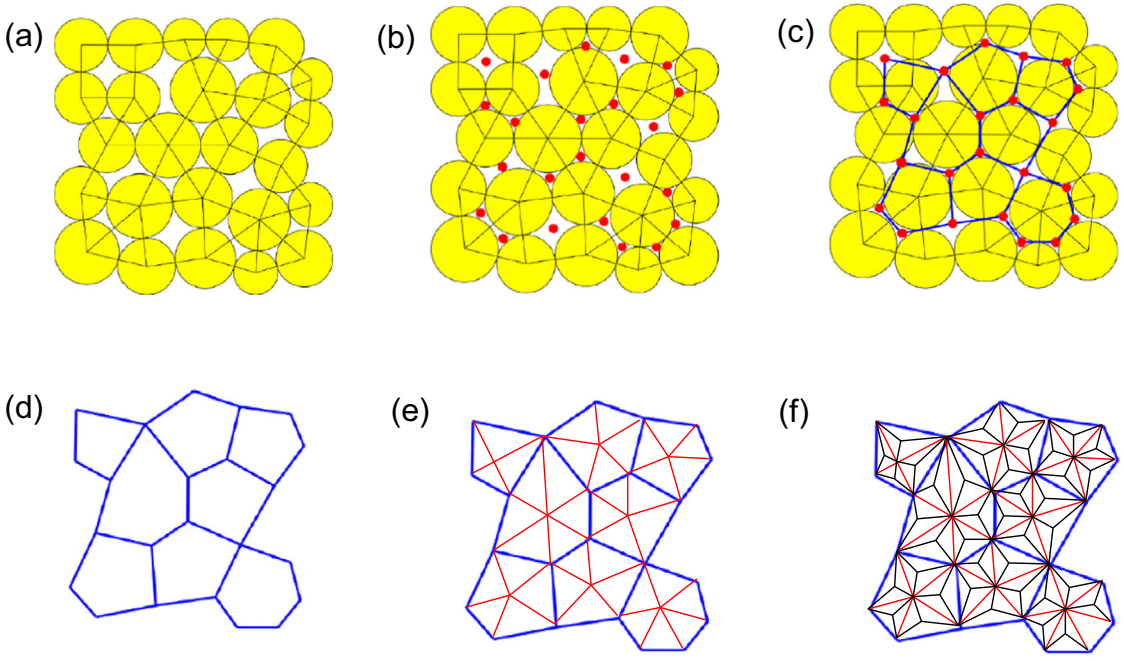

Fig. 1. Grain structure generation. (a) Initial disk packing; (b) void centroids (red dots); (c) polygonal network; (d) grain structure; (e) intra-grain bonds (red lines) and (f) further discretization (black lines) (a–d from [16]). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)