Computers and Geotechnics 103 (2018) 73–81

Contents lists available at ScienceDirect

Computers and Geotechnics

journal homepage: www.elsevier.com/locate/compgeo

Research Paper

Grain based modelling of rocks using the combined finite-discrete element method

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ARTICLE INFO

Keywords:
Grain based modelling
Combined finite-discrete element method
Microscopic and macroscopic rock behaviour

ABSTRACT

This paper describes the implementation and advantages of grain based modelling (GBM) in the combined finite-discrete element method (FDEM) to study the mechanical behaviour of crystalline rocks. GBM in FDEM honours grain petrological properties and explicitly models grain boundaries. The simulation results demonstrated that GBM in FDEM predicted more realistic microscopic and macroscopic response of rocks than conventional FDEM models. The explicit modelling of crack boundaries captured microscopic failure transition from along grain boundaries to coalescence along the shear band, dominated by intraphase cracks. This novel framework presents a gateway into further understanding the behaviour of crystalline rocks and granular minerals.

1. Introduction

Macroscopic behaviour and bulk properties of crystalline rocks are closely related to their microstructures, which are characterized by the grain scale properties [1,2]. These properties include grain morphology, grain size and spatial distribution, crystallographic anisotropy and orientation, elastic properties of grains, and the properties of the grain interfaces [2]. Thus, investigation of the rock microstructural failure considering grain scale behaviour is of fundamental importance to determine the macroscopic response of the rock (e.g. stress-strain response), the localized microscopic phenomena (e.g. nucleation and propagation of cracks), and their sensitivity to the presence of bedding planes, flaws, pores, and cavities [3].

The Griffith theory assumes that the propagation and coalescence of the existing flaws in the material fabric is the source of macroscopic failure [4]. Petrographic studies have demonstrated that different processes, natural or stress-induced, produce cracks with peculiar and recognizable characteristics [5,6]. However, crack initiation, crack propagation, and specimen failure are progressive and separate processes [7]. In rocks, microcracks form when the local stress exceeds the local strength, and the coalescence of many microcracks forms macroscopic fractures with some crack configurations being more favourable for coalescence than others [5]. Kranz [5] categorizes microcracks in rock into four types: grain boundary cracks (coincident with a grain boundary), intragranular cracks (cracks lie totally within the grain and do not extend to a grain boundary); intergranular cracks (cracks which extend from a grain boundary to another grain boundary); and multigranular or transgranular cracks (cracks which cross several grains and grain boundaries). Eberhardt et al. [8] have shown that the grain size has a minor effect on the stress at which cracks initiate, but their effect is significant in controlling the behaviour and trajectory of the propagating crack, which in turn influences the macroscopic fracture propagation. In addition, the strength of the mineral constituent and their cementation have a significant effect on crack initiation [7,8].

Laboratory experimental studies of grain deformation and crack mechanisms are exhaustive and very complicated procedures. In addition, experimental results are dictated by sample specific characteristics, such as naturally occurring grain morphologies and orientations, which makes experimental repeatability nearly impossible. One way to overcome these limitations is the use of a modelling technique that can account for specific morphologies and microstructure crystal shape and distribution. Voronoi tessellations (i.e. Voronoi diagrams), which are considered suitable representations of polycrystalline granular structures [9], have been proposed to address this point in numerical simulations. For example, in the Particle Flow Code grain based models (PFC2D-GBM) developed by Potyondy [10], Voronoi-like diagrams are generated using clumped circular particles to represent grains and smooth-joint contacts to represent the grain interfaces [11–15]. In the Universal Distinct Element Code (UDEC), the grain based models (GBM) are initially created using the PFC-GBM packing scheme [10], and the resulting Voronoi-like diagram is used to generate blocks. These blocks represent grains and their contact surface represent the grain interface. The generated blocks can be unbreakable [16,17] or sub-divided into several smaller blocks to account for breakable grains [18–20]. The

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https://doi.org/10.1016/j.compgeo.2018.07.003
Received 9 October 2017; Received in revised form 3 July 2018; Accepted 3 July 2018
0266-352X/

UDEC-GBM, with the contact along the grain boundary, overcame some of the limitations of PFC2D-GBM approach in representing rock-like morphologies; however, both approaches used a single bond strength to represent the various grain interfaces.

Conventional simulations in the combined finite-discrete element method (FDEM) attempted to simulate heterogeneous models using unstructured 2D Delaunay triangulation models (i.e., each triangulation represented a mineral phase) to represent sample heterogeneity [21–23]. Those models were not intended to mimic the effect of grains but rather identify the effect of heterogeneity on rock failure behaviour; thus, were unable to investigate the role of intergranular and intragranular cracks.

In this paper, we introduce a novel Voronoi diagrams based approach to realize grain based modelling (GBM) in the combined finite-discrete element method (FDEM). This framework enables the explicit modelling of the intergranular and intragranular contacts between the various grains, while also taking into consideration the actual grain morphology. Furthermore, this explicit modelling approach allows each grain contact to be assigned different properties, whether the contact is between dissimilar grains (i.e. interphase boundary) or similar mineral phases (i.e. homophase boundary).

This paper is structured to initially introduce the microstructure modelling and the new algorithm developed for GBM, followed by a discussion that validates the simulation results against published experimental results [23] and numerical studies [21]. Then we present the advantages of GBM over conventional FDEM micro-modelling approaches [21,23–25]. GBM provides an efficient way to model fracturable mineral grains to provide insights into grain scale crack propagation and crack patterns, and to enhance the understanding of the relationship between the evolution of the stress-strain curve and the failure mechanisms of crystalline rocks.

2. Concepts and methods

2.1. The combined finite-discrete element method (FDEM)

FDEM was first introduced by Munjiza et al. [26] to simulate the behaviour of deformable bodies and their interactions. The method was further developed to simulate rock behaviour by explicitly modelling rock elastic deformation, crack initiation, and crack propagation [27]. A two-dimensional (2D) FDEM model is built based on a discretized triangular element mesh (Fig. 1), where each adjacent pair of triangular elements is connected with a four-node cohesive crack element (CCE) (Fig. 1) [28,29].

The CCE undergoes elastic deformation according to the stress conditions, and once the stress within the elements overcomes the intrinsic strength of the material, the displacement-based yielding and failure process initiates [27]. This process is simulated by explicitly modelling crack initiation and propagation using softening and breakage of the CCE, allowing the model to transition from a continuum to discontinuum (Fig. 1) [22,27]. As the simulation progresses, finite displacements and rotations of the discrete bodies are allowed and new contacts are recognized [27].

2.2. Voronoi diagrams

Voronoi diagrams are extensively used in computational geometry and have been already adopted for representing polycrystalline materials at the grain scale [1,9,30]. Voronoi diagrams have several distinct advantages: first, they can be defined analytically and numerically to possess unique geometrical properties; secondly, the polygons are a convex set that they are confined in the domain in which they exist (i.e. collectively exhaustive as every point within the domain is assigned to a seed); and lastly, they are mutually exclusive except for their boundaries (i.e. two adjacent tessellations do not overlap but share a boundary). These unique geometrical properties translate into Voronoi diagrams being an adequate morphological generator for polycrystalline structures as the grains fill up the entire domain; furthermore, the seeds are fixed at their spatial position during the growth process resulting in no overlapping between the grains [1,31–33]. Adaptation of such modelling techniques can help evaluate the impact of the morphological changes and mineral grain properties on crack initiation and crack propagation.

In this work, Voronoi diagrams (Fig. 2a) are created from points (Voronoi seeds) placed inside defined domains using a Poisson random point process [33]. An edge in Voronoi diagrams is created by constructing a perpendicular bisector to the line connecting two adjacent Voronoi seeds. The line connecting the intersections of these lines (i.e., Voronoi vertex) encloses the initial region. With the initial regions established, a regularization process removes all the small edges of the Voronoi regions smaller than a user defined value (e.g. smallest grain size). Removing these small edges can reduce the pathological behaviour of the subsequent mesh of the FDEM model and avoid the need of excessive mesh refinement. However, it also causes geometric distortion, which is resolved by a two-step process: new vertex positioning and new region interpolation [33]. Fig. A1 in the Appendix illustrates the 2D regularization process. This process is iterative and terminates when all edges meet the defined threshold, or when the maximum number of user defined regularization loops has been reached.

3. GBM in FDEM

3.1. Grain and grain boundary modelling

Minerals exist in various crystal forms that are determined by factors such as the crystal structure (internal factors), and the condition of the crystal growth process (external factors, e.g. temperature and pressure). Voronoi tessellations can be used to numerically reproduce

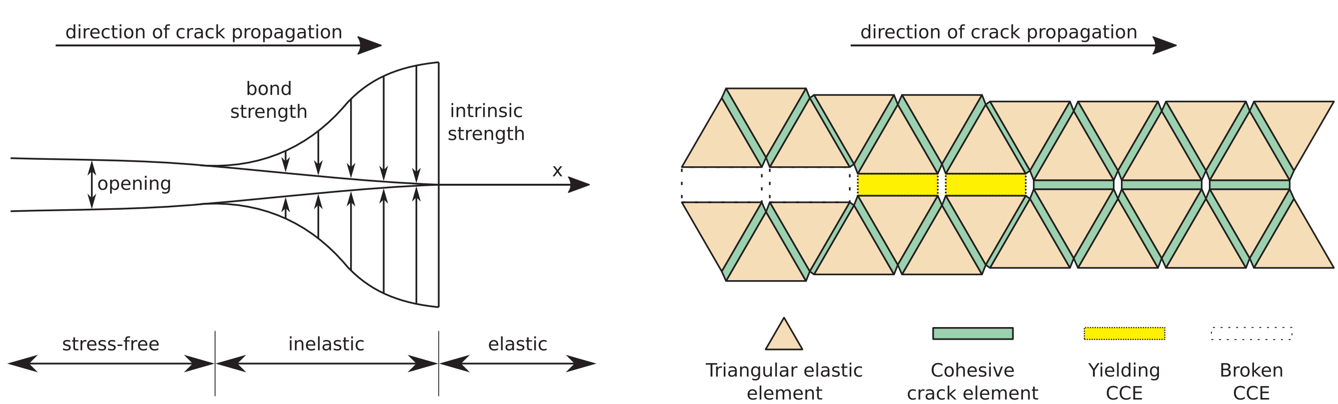

Fig. 1. Typical behaviour of cohesive crack elements in FDEM (adapted from Lisjak et al. [22]).