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On the suitability of a Discrete Element Method to simulate cracks initiation and propagation in heterogeneous media

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ABSTRACT

The present paper investigates the suitability of a Discrete Element Method (DEM) to simulate cracks initiation and propagation in heterogeneous media. We focus our studies on the cohesive hybrid-particulate model in which the continuous medium is modeled using a cohesive beam model. Previous works exhibited the ability of such an approach to simulate the mechanical behavior of continuous materials under various solicitations. The DEM is actually well-suited to take into account local heterogeneities and complex fracture phenomena occurring at very fine scales. In a first step, several tests are performed in the context of a 2D homogeneous medium in order to better quantify micro-macro scale transition effects related to the DEM on cracks initiation and propagation. Then, in a second step, unidirectional fibre-reinforced composites are modeled using 2D models taking into account a brittle matrix failure and interfacial debonding effects. Numerical tensile tests are set up for two main configurations: a single-fiber composite constituted of a single fiber embedded in an alumina matrix and the case of multi-fiber composites constituted of parallel fibers also embedded in an alumina matrix. The results exhibit the suitability of the DEM to yield suitable stress fields and crack patterns in the investigated heterogeneous media. Scale transition effects are noticeable in terms of stress fields but turn out to be relatively limited in the mechanism leading to cracks initiation and propagation. Furthermore, the competition between debonding and failure is also well captured whatever the fiber arrangement.

1. Introduction

Characterized by an excellent stiffness-to-weight ratio, a good flexibility, a potential high strength and the ability to resist to corrosion, composite materials have become widely used in many industrial sectors such as aeronautic, aerospace, automotive, building and marine. Besides, the development of biocomposites composed of a polymer matrix potentially derived from renewable resources and natural fibres as flax or hemp has paved the way to new materials able to respond to current sustainability and environment issues. However, in order to make them able to serve specific purposes in various situations, their performance and safety have to be thoroughly monitored. Thus, the composite has to resist to time degradation and fatigue under a large scope of solicitations. This requires an accurate multi-scale characterization of the material to better understand the process leading to damaging. For this purpose, in order to replace long and costly experimental measurements, the development of robust numerical methods has become a scientific challenge of main interest. These aim to better characterize the mechanical behavior of composites and the phenomena arising in the material such as crack initiations, interfacial debonding, defect effects, local variability and heterogeneity.

From a numerical standpoint, several methods exist for simulating cracks initiation and propagation. Most of them are based on the Finite Element Method (FEM) which can be extended to embed the discontinuity. Thus, the eXtended Finite Element Method (XFEM) (Moës et al., 1999) was initially set up to tackle the difficulties related to the mesh updating and is now used for a larger scope of applications. However, such an approach is poorly adapted to model multiple fractures with joining and bifurcating cracks due to costly crack path enforcement. Other methods only allow cracks to propagate between the elements. For example, the Virtual Crack Closure Technique (VCCT) is often considered for modeling and predicting the delamination (Krueger, 2004). Other approaches such as the Cohesive Zone Model (CZM) (Xu and Needleman, 1994; Zhang and Paulino, 2005) and its variants the Discrete Cohesive Zone Model (DCZM) (Xie and Waas, 2006) and the Discrete Damage Zone Model (DDZM) (Liu et al., 2012) give the possibility to consider random crack initiation and to manage

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multiple cracks propagation in the material. These methods are mesh-dependent and require a costly remeshing to alleviate these effects. Other approaches which can be qualified as meshless methods enable to consider crack propagation without representation of the crack's topology. Thus, the cracking particles method introduced by Rabczuk and Belytschko (2004); 2007) and later improved to avoid local enrichment (Rabczuk et al., 2010) uses a continuous description of the medium coupled to a discrete representation of the discontinuity. Its advantage is to more naturally treat complex crack propagation but this is a priori less accurate than methods based on embedded elements. Peridynamics (Silling, 2000) and its variants as the dual-horizon peridynamics (Ren et al., 2016) use a continuous description based on an integral formulation in order to avoid classical issues related to partial differential equations. In this approach, forces applied to a particle are estimated by summing the contributions of a set of surrounding particles located in an area called horizon. Another class of methods based on a particulate system also exists. Originally used in the field of rock mechanics (Cundall and Strack, 1979; Cleary and Campbell, 1993), the DEM is an ideal tool for solving mechanical problems in which multiple scales and discontinuities arise. This approach exhibits several similarities with the peridynamics since the motion of a particle is also computed by summing the forces of neighboring particles. However, the DEM uses a discrete representation in the sense that all particles have to be modeled as individual entities and requires to calibrate microscopic parameters.

In the last decade, the DEM was used in various domains among them the simulation of tribological granular flows (Fillot et al., 2007), silo discharge (Nicot et al., 2013), impact effects on concrete (Shiu et al., 2008), vickers indentation (Jebahi et al., 2013) and ball bearing loading (Machado et al., 2015). Besides, the DEM was also considered for simulating cracks initiation and propagation in continuous materials (Hentz et al., 2004; Tan et al., 2009; André et al., 2013). In this domain, the most important challenge was to develop a numerical model able to quantitatively reproduce the multi-scale mechanical behavior of a continuous medium. Based on the works of Schlangen and Garboczi (1997), it was established that the cohesive beam model (André et al., 2012) is more suitable than spring elements to model continuous media and its damaging under several mechanical loadings. Furthermore, recent works highlighted the ability of the cohesive beam model to simulate the mechanical behavior of heterogeneous materials throughout the examples of a unidirectional fibre composite (Maheo et al., 2015) and random media (Haddad et al., 2015). The issue of cracks initiation and propagation in composites was partially treated by Le et al. (2016) in the field of composite fibres. However, the authors only considered the cohesive beam model for modeling the matrix phase and more in-depth studies have to be performed to relate the mechanical behavior to the process leading to damaging and cracks propagation.

In the present work, we aim to investigate the suitability of the cohesive beam model to simulate cracks initiation and propagation in heterogeneous media. Besides, we intend to better understand the influence of variability effects related to the micro-macro scale transition in the Discrete Element (DE) approach on the damaging initiation and the crack propagation. For this purpose, we consider the Removed DE Failure (RDEF) criterion introduced by André et al. (2013). We suppose a brittle fracture with a mode I crack propagation so that damaging occurs when the hydrostatic stress is greater than a given stress limit. Interfacial debonding effects are also taken into account by the DDZM introduced by Liu et al. (2012) and here adapted for discrete simulations. In a first step, several tests are performed in the context of a 2D homogeneous material in order to better exhibit the micro-macro scale transition effects on the damaging process and their influence on crack propagation. Thus, a plate with a centered hole, a 3-point bending test and an indentation test are modeled and studied. In each case, the variability is observed using stress fields determined using Zhou's formulation (Zhou, 2003) at the scale of the particle and using Love-Weber formulation (Nicot et al., 2013; Love, 1927) at a mesoscale introduced with the help of a tessellation of the domain in specimen (Nicot et al., 2013; Haddad et al., 2015). In a second step, we investigate the case of composite materials. Two main models are considered: a composite composed of a single metallic fiber embedded in an alumina matrix and the case of parallel metallic fibers randomly embedded in an alumina matrix. In this latter example, effects related to the arrangement of fibres are also considered using closely-packed and dilute fiber arrays. In each configuration, tensile tests are modeled and the positive part of the hydrostatic stress field is observed before, during and after the crack initiation. For sake of clarity, only the matrix failure is considered and fibers are supposed undamageable for each investigated case. Cracks propagation, variability effects, and the competition between matrix failure and interfacial debonding are finally discussed.

The paper is organized as follows. Section 2 is dedicated to the DEM based on the cohesive beam model which is designated as the Cohesive Discrete Element Method (CDEM) in the sequel for more conciseness. Section 3 introduces the RDEF criterion describing the matrix failure and the DDZM simulating the interfacial debonding. Section 4 deals with the three numerical tests carried out in the context of a homogeneous medium. Finally, Section 5 is dedicated to the modeling of tensile tests carried out on representative patterns of composite materials.

2. CDEM

The present section describes the CDEM as developed by Haddad et al. (2015) in 2D and André et al. (2012) in 3D. In this approach a continuous medium is modeled by a granular packing consisted of disks in point contact in 2D (spheres in 3D) in which the cohesion between two particles is itself modeled by a beam element. Under several assumptions of size and isotropy, the obtained hybrid particulate-lattice model can be designated as an Equivalent Continuous Domain (ECD) the mechanical properties of which are related to those of beam elements using a calibration process.

2.1. ECD

The CDEM is based on the discretization of a continuous medium by a granular packing composed of disks in point contact in 2D. In the present work, granular packings are generated by the efficient Lubachevsky–Stillinger Algorithm (LSA) (Lubachevsky and Stillinger, 1990) which enables an accurate control of intrinsec parameters such as the compacity, the polydispersity, the coordination number and the randomness of contact angles. Under several assumptions related to these parameters, the granular domain can be then considered as an ECD in that this is enough representative of the continuous medium. First, the compacity in terms of volume fraction has to be closed to 0.85 which corresponds to the Random Close Packing (RCP) (Torquato et al., 2000; Donev et al., 2004) for a random granular packing composed of circular particles in 2D. Second, the coordination number which represents the average number of particles in contact with one given particle has to be close to 4.5. Third, a slight polydispersity of particle size must be introduced in order to avoid undesirable directional effects. Typically, the particle's radius follows a Gaussian distribution law and the dispersion is characterized by the coefficient of variation which is the ratio between the standard deviation and the average radius. For information purposes, this is set to 0.3 in the present work.