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Adaptive concurrent multiscale model for fracture and crack propagation in heterogeneous media

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Abstract

We introduce an adaptive concurrent multiscale methodology (ACM^2) to handle situations in which both macroscopic and microscopic deformation fields strongly interact near the tip of a crack. The method is based on the balance between numerical and homogenization error; while the first type of error states that elements should be refined in regions of high deformation gradients, the second implies that element size may not be smaller than a threshold determined by the size of the unit cell representing the material's microstructure. In this context, we build a finite element framework in which unit cells can be embedded in continuum region through appropriate macro–micro boundary coupling conditions. By combining the idea of adaptive refinement with the embedded unit cell technique, the methodology ensures that appropriate descriptions of the material are used adequately, regardless of the severity of deformations. We will then show that our computational technique, in conjunction with the extended finite element method, is ideal to study the strong interactions between a crack and the microstructure of heterogeneous media. In particular, it enables an explicit description of microstructural features near the crack tip, while a computationally inexpensive coarse scale continuum description is used in the rest of the domain. The paper presents several examples of crack propagation in materials with random microstructures and discuss the potential of the multiscale technique in relating microstructural details to material strength and toughness.

Keywords: Concurrent multiscale method; Adaptivity; Strain localization; Damage and fracture; Heterogeneous media

1. Introduction

Today's technological advances in micro- and nanofabrication will soon enable the design of new materials that are sustainable, durable and multifunctional through a careful control of their micro-architecture. Proof-of-concepts have already been provided by a number of biological materials that, due to their highly organized microstructure, overwhelmingly exhibit a high fracture toughness, despite their weak building blocks [15].

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Fracture resistance is also particularly desirable for next generation of synthetic materials. However, unlike biological materials, they do not benefit from the efficient, but lengthy evolution process to optimize their properties. The development of man-made materials must therefore rely on the use of rational design and mathematical modeling to accurately describe material failure and subsequently predict microstructures that can resist failure the most. So far, research efforts have been hindered by the fact that fracture mechanics in heterogeneous media typically involve two distinct and separate length-scales. On the one hand, the growth of a ductile crack occurs via the evolution of damage ahead of the crack tip, in a relatively small region, known as the process zone [61,2]. In this region, materials usually exhibit a complex behavior involving inelasticity, damage and eventually a strain-softening response that may induce size effects [2,33]. A micromechanical modeling approach [37] is often necessary to accurately capture these mechanisms and their effects on fracture resistance. On the other hand, fracture initiation and propagation highly depends on macroscopic loading, geometry and macroscopic material features. At this level, a continuum description is usually preferred due to its ability to describe uniform material deformation and its low computational cost. Because of this scale separation, theoretical studies on the role of microscopic damage on fracture properties have been limited to either unrealistically small domains or overly restrictive assumptions. Instances include the studies of ductile crack growth in metallic alloys [45,39,60], or numerical predictions of the fracture resistance of biological silica-based composites [47], to name a few.

From a theoretical and computational viewpoint, a number of alternative strategies have been proposed to address the multiscale dilemma. For instance, a potential solution was provided by the development of higher order continuum theories such as micromorphic theories [61,59,60], micro-continuum models [56,19], Cosserat theory [9,13,24] or strain gradient theories [23,22,14] in order to capture microstructural size effects when the material deformation becomes inhomogeneous. These methods have been particularly successful when the displacement fields are nonuniform, but smooth, such as during plasticity and the early stages of material's failure. However, when the deformation fields become strongly non-uniform and non-smooth, the very validity of continuum assumptions becomes questionable and new approaches must be considered. In this context, the use of microstructural descriptions provide a clear solution but they often involve computational problems that are intractable over domains of realistic size. This has motivated the development of multiscale methods that can bridge microstructural material descriptions (in regions in which highly heterogeneous deformation occurs) and the continuum description (where the deformation field is homogeneous) [40,30]. For instance, a class of concurrent multiscale methods [41,32,62,6] was introduced based on the idea that a microscopic region can be determined a priori (such as around a crack tip) and coupled with a coarse grained continuum region via appropriately designed bridging scale conditions. Using a similar idea, Ghosh et al. [26,25], Moorthy and Ghosh [35], and Raghavan and Ghosh [44,43] introduced a method based on Voronoi Cell Finite Element Method (VCFEM) to deal with problems in which the microscopic region is not a priori determined but is informed by the nature of the numerical solution. Finally, we have previously introduced a finite element based adaptive concurrent multiscale method (ACM^2) that provided a dual (micro–macro) description of an elasticity problem by adaptively splitting a physical domain into a microstructural component (with refined description) and macroscopic continuum component [20]. The adaptivity of the method relied on the idea that element refinement should result from two kinds of approximation errors: discretization and homogenization. This led to the idea that continuum finite element description can only be refined up to a certain level after which elements must be replaced by a more refined microstructural description provided by so-called unit cells.

Despite the number of powerful methods, establishing a relationship between microstructure and the mechanisms of damage evolution and crack propagation still remains a challenge. We therefore propose to extend the concepts behind the ACM^2 to address this shortcoming. The contributions of this paper are several folds. First, we present a method for which a crack is naturally accounted for at both micro and macro scales by coupling the aforementioned multiscale technique with the extended finite element method. Second, because strain and rotation fields are often large in the vicinity of the tip of a loaded crack, we present an iterative nonlinear formulation of the ACM^2 for finite deformation and nonlinear material response. Third and finally, we account for damage nucleation and evolution in the crack tip region by modeling the microscopic material response with a lattice model. This feature is critical to capture the phenomenon of crack propagation in heterogeneous materials. We show, via a variety of examples, that the ACM^2 enables both continuum and explicit