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A phase field method to simulate crack nucleation and propagation in strongly heterogeneous materials from direct imaging of their microstructure

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ABSTRACT

In this work, crack initiation and propagation in 2D and 3D highly heterogeneous materials models, such as those obtained by micro-CT imagery of cementitious materials, is investigated for the first time by means of the phase field method. A shifted strain split operator algorithm is proposed to handle unilateral contact within cracks in a very efficient manner. The various advantages of the phase field method for voxel-based models are discussed. More specifically, we show that the resolution related to the initial image and thus to meshes for discretizing the same microstructure does not significantly affect the simulated crack path.

1. Introduction

The numerical simulation of crack propagation in highly heterogeneous materials is a very challenging problem. Recently, the use of experimental techniques such as X-ray microtomography [19] has allowed to construct realistic microstructural models of material like concrete, biological tissues (cortical bones), or composites, among many others. Developing damage models for these highly heterogeneous materials taking into account the real microstructure offers new avenues to predict more accurately fracture processes in related structures and is of formidable interest in engineering.

Unfortunately, because of the possible occurrence of multiple arbitrary branching cracks in such materials, several obstacles remain to develop reliable simulation methods of fracture nucleation and propagation in highly complex heterogeneous materials. On one hand, the classical treatment of quasi-static and dynamic fracture based on the classical Griffith theory [24,22,25,26] fails to describe crack nucleation or crack branching. Furthermore, the sharp representation of cracks requires the identification of a crack growth law, which is a complex task in the general case. On the other hand, many numerical simulation methods for crack propagation have been developed in the recent decades, but each faces well-known issues and drawbacks: (i) direct tracking of the crack front, using classical theory of brittle fracture, requires very complex remeshing algorithms [30], which are hardly tractable for complex 3D morphologies, or multiple crack fronts. The problem can be alleviated by means of recent local/global meshes superposition [33]; (ii) classical smeared crack models [32,51] suffer from inherent mesh sensitivity, which can be partially circumvented with nonlocal averaging schemes [49], or implicit gradient

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Nomenclature

d	phase field variable
l	regularization parameter
E	total energy of the body
W	free energy
W_u	elastic strain energy density function
g_c	fracture toughness
$\mathbf{u}$	displacement vector
$\boldsymbol{\varepsilon}$	linearized strain tensor
$\boldsymbol{\sigma}$	Cauchy stress tensor
γ	crack density function
Γ_l	total crack length
ϕ	dissipation function
$\mathcal{A}$	thermodynamic force associated with d
Ψ^+	strain energy density function associated with extension mode
Ψ^-	strain energy density function associated with compression mode
$\boldsymbol{\varepsilon}^+$	extension part of the strain tensor
$\boldsymbol{\varepsilon}^-$	compression part of the strain tensor
λ	Lamé's coefficient
μ	shear coefficient
$\mathcal{H}$	strain history functional
$\mathbb{P}^+$	projection tensor such that $\boldsymbol{\varepsilon}^+ = \mathbb{P}^+ : \boldsymbol{\varepsilon}$
$\mathbb{P}^-$	projection tensor such that $\boldsymbol{\varepsilon}^- = \mathbb{P}^- : \boldsymbol{\varepsilon}$
Δt	time step

models [47]; (iii) methods relying on local enrichment to avoid remeshing, like the extended finite element method (XFEM) [43,5,18] require the use of a level-set function [46] to describe the geometry of the crack, inducing difficulties for crack nucleation, crack branching, and is very cumbersome for multiple crack fronts. Applications and developments of XFEM for 3D fracture problems can be found e.g. in [44,23,55,29] and in [28] in a multiscale framework; (iv) cohesive elements (see e.g. [57,15,58]) can deal with multiple crack fronts and crack nucleation, but imply the cracks to follow the elements, and suffer from convergence issues with refined meshes; finally (v), we mention a new method, called Thick Level-Set method (TLS) [7,16] in which a level-set function is employed to separate the undamaged zone from the damaged one, and where the crack is a consequence of the damage front motion, allowing crack initiation.

Recently, a new approach for the description of crack propagation has been developed. Starting from the pioneering works of Francfort and Marigo [20], difficulties arising in the classical fracture framework can be overcome by a variational-based energy minimization framework for brittle fracture (see also [10,48,9,14,4]). An important ingredient of the method relies on a regularized description of the discontinuities related to the crack front: the surface of the crack is replaced by a smooth function, using a Mumford–Shah functional [45], the original functional being substituted by an Ambrosio–Tortorelli approximation [2,3]. It has been shown that the solution of the associated variational problem converges to the solution of the sharp crack description implying discontinuities, in the Γ-convergence sense [36,12,13]. The approximation then regularizes a sharp crack surface topology in the solid by a scalar auxiliary variable, interpreted as a phase field describing broken and unbroken parts of the solid. Such a method has the quality that it does not require any prescription of the shape geometry and allows crack nucleation and branching, providing a very robust framework for crack propagation simulation. It has been adapted to quasi-static fracture problems in [9,8], dynamic crack propagation [11,27], and in a multiphysic context in [39,1]. Remarkably, the regularized model may be regarded as a damage model of the gradient type [34,35,6,47,21] with critical differences in the choice of the free energy and dissipation function. Recently, the problem of cohesive fracture has been reformulated in the context of phase field [56].

In this work, crack propagation in highly heterogeneous microstructures, such as segmented X-ray CT images of real materials, which are used as direct input of the simulations, is investigated for the first time by means of the phase field method, which here follows the algorithmic framework proposed by Miehe et al. [37,40]. To increase the computational efficiency of the method, a modified shifted algorithm has been introduced, to compute the strain tensor split, leading to a very simple and fast algorithm. The advantages of such an approach are demonstrated for crack nucleation and propagation in voxel-based models. Several applications to 2D and 3D images of porous cement-based materials are provided.

The overview of the paper is as follows. In Sections 2 and 3, the main idea and thermodynamic foundations of the phase field method such as presented in Miehe et al. [37,40] are reviewed. In Section 4, the computational and algorithmic framework based on finite elements is presented. A shifted strain tensor split algorithm is introduced to simplify the treatment of damage, assumed to be only induced by the tensile strain, to provide an efficient algorithm. Finally, numerical examples are presented in Section 5.