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Phase field modeling of quasi-static and dynamic crack propagation: COMSOL implementation and case studies

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ABSTRACT

The phase-field model (PFM) represents the crack geometry in a diffusive way without introducing sharp discontinuities. This feature enables PFM to effectively model crack propagation compared with numerical methods based on discrete crack model, especially for complex crack patterns. Due to the involvement of "phased field", phase-field method can be essentially treated a multifield problem even for pure mechanical problem. Therefore, it is supposed that the implementation of PFM based on a software developer that especially supports the solution of multifield problems should be more effective, simpler and more efficient than PFM implemented on a general finite element software. In this work, the authors aim to devise a simple and efficient implementation of phase-field model for the modelling of quasi-static and dynamic fracture in the general purpose commercial software developer, COMSOL Multiphysics. Notably only the tensile stress induced crack is accounted for crack evolution by using the decomposition of elastic strain energy. The width of the diffusive crack is controlled by a length-scale parameter. Equations that govern body motion and phase-field evolution are written into different modules in COMSOL, which are then coupled to a whole system to be solved. A staggered scheme is adopted to solve the coupled system and each module is solved sequentially during one time step. A number of 2D and 3D examples are tested to investigate the performance of the present implementation. Our simulations show good agreement with previous works, indicating the feasibility and validity of the COMSOL implementation of PFM.

1. Introduction

Fracture induced failure has obtained extensive concern in engineering designs because of the potential serious risks for structures and machines being used [1]. The research on crack initiation and propagation in solids has therefore become very important [2]. Particularly, when experiments are difficult, or even impossible to perform for studying certain type of crack propagation, researchers have to employ numerical approaches to predict complicated crack paths [3] such as those in multiple scales [4–8]. Consequently, a great number of numerical methods have been proposed to deal with crack problems in recent years.

Most of these methods have to describe complex crack geometry in the discrete setting, such as the discrete crack models [9], the extended finite element method (XFEM) [10,11], generalized finite-elements method (GFEM) [12], and the phantom-node method [13,14]. These methods all enrich the displacement field with discontinuities. Particularly, the discrete crack model [9] introduces new boundaries for the freshly created crack surfaces by an adaptive reconstruction of the mesh. XFEM [10] enriches the cracked elements by adding a set of discontinuous shape functions to the standard parts of FEM. Another common option to model cracks is the so-called cohesive elements [15–17] that allow displacement jumps on element boundaries and cracks are therefore restricted to penetrate along the corresponding element edges. In addition, the element-erosion methods [18–20] also succeeds in dealing with the fracture surfaces by setting the stresses of the elements, which meet the fracture criterion, as zero. However, the element-erosion methods have the disadvantage that they cannot simulate crack branching correctly [21]. Therefore, the complicated and special treatments for complex crack topologies have made these numerical approaches not so easy to implement and apply in practical engineering.

A recently emerged and developed approach, the phase-field method (PFM) [22–26], has attracted a lot of attention because of its

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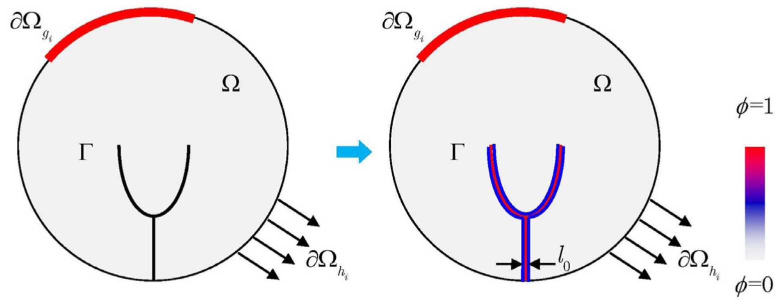

Fig. 1. Phase-field approximation of the crack surface.

relatively easier numerical implementation for fracture. The phase-field models utilize a scalar field (so-called phase-field) to represent the discrete cracks. The phase-field does not describe the crack as a physical discontinuity and just smoothly transits the intact material to the thoroughly broken one. The shape and propagation of the crack depend on the evolution equations of the phase-field. Thus, implementation of the phase-field does not require additional work to track the fracture surfaces algorithmically [24]. This results in that the phase-field methods have a large advantage over the discrete fracture models for modeling multiple and crack branching and merging in materials with arbitrary 2D and 3D geometries.

The phase-field models for quasi-static brittle crack started from [27] and improved by authors in [22,23]. All these models are regarded as extension of the classical Griffith fracture theory and then extended to dynamic problems by Borden et al. [24]. In addition, Landau–Ginzburg type evolution equations [28] instead of the Griffith type have also been proposed and developed for the phase-field description of dynamic fracture. The progress in the phase-field models for quasi-static and dynamic crack problems has made PFM successfully applied in different problems, such as cohesive fractures [29], ductile fractures [30,31], large strain problems [25], hydraulic fracturing [32], thermo-elastic problems [33,34], electrochemical problems [35], thin shell [36], and stressed grain growth in polycrystalline metals [37–39]. These attempts imply that the application of the phase-field methods is quite beyond purely mechanical problems. This naturally requires a much easier implementation approach for the phase-field models. Otherwise, extensive application of the phase-field models will be restricted, especially in multi-physical problems.

Due to the smooth characteristics of the phase-field, the phase-field method can be implemented in any existing standard finite element to model complex crack patterns as shown in [22,23]. Therefore, to reduce the efforts in implementation, it is desirable to implement phase-field method to an extensively used FEM code or commercial software. In fact, [40] and [2] have implemented the phase-field method for brittle cracks in Abaqus. However, the phase-field modeling itself is essentially a multi-field problem even in the case of pure mechanical problem [22,23]. From the authors' experience, it is laborious and time consuming to implement a multifield problem in Abaqus. Therefore, a general purpose programme developer that especially supports the programming of multifield problem such as COMSOL has the potential to become a better solution than Abaqus.

In this paper, the possibility of simple and fast implementation of phase-field method is exploited for fracture modelling in a multifield programme developer, namely COMSOL Multiphysics. The phase-field modeling in COMSOL can be easily extended to problems that have more coupled fields by just adding suitable modules and coupling terms. It will be quite easy for readers to use this first-step implementation and augment it by other physical phenomena to solve multiphysics problems involving crack propagation. For example, the phase field implementation in COMSOL can be extended and applied to hydraulic fracturing, or compressed air energy storage [41,42], which involves fluid pressure field, temperature, and cyclic effects [43–46]. In this work, one phase-field model presented by authors in [22,23] for a quasi-static crack problem and another one presented by Borden et al. [24] for dynamic problems are implemented in COMSOL in a staggered scheme. The elastic strain energy density is decomposed into two individual parts resulting from compression and tension, respectively. Thus, the fractures only due to tension can be obtained. In COMSOL, we use an implicit time integration scheme to enable the simulation. We also calculate some 2D and 3D benchmarks for quasi-static and dynamic crack propagation to show the feasibility of our approach for modeling fracture.

The paper is organized as follows. We begin with a short introduction of the phase-field model for brittle fractures based on the variational approach in Section 2. Subsequently, we present the numerical implementation of the phase-field model in COMSOL in Section 3. In Section 4, we examine some 2D and 3D numerical examples for cracks under quasi-static and dynamic loading. Finally, we end with conclusions regarding our findings in Section 5.

2. Phase-field model for fracture

2.1. Theory of brittle fracture

Let us consider an arbitrary body $\Omega \subset \mathbb{R}^d$ $(d \in \{1, 2, 3\})$ as shown in Fig. 1. The body Ω has an external boundary $\partial\Omega$ and internal discontinuity boundary Γ. The displacement of body Ω at time t is denoted by $\boldsymbol{u}(\boldsymbol{x}, t) \subset \mathbb{R}^d$ where $\boldsymbol{x}$ is the position vector. The displacement field satisfies the time-dependent Dirichlet boundary conditions, $u_i(\boldsymbol{x}, t) = g_i(\boldsymbol{x}, t)$, on $\partial\Omega_{g_i} \in \Omega$, and also the time-dependent Neumann conditions on $\partial\Omega_{h_i} \in \Omega$. We also consider a body force $\boldsymbol{b}(\boldsymbol{x}, t) \subset \mathbb{R}^d$ acted on the body Ω and a traction $\boldsymbol{f}(\boldsymbol{x}, t)$ on the boundary $\partial\Omega_{h_i}$.

A variational approach for fracture problems according to Griffith's theory has been proposed in [47]. It states that the required energy to create a fracture surface per unit area is equal to the critical fracture energy density G_c, which is also commonly referred to as the critical energy release rate. The total potential energy $\Psi_{opt}(\boldsymbol{u}, \Gamma)$ can be expressed in terms of the elastic energy $\psi_\varepsilon(\boldsymbol{\varepsilon})$, fracture energy and energy due to external forces:

$$\Psi_{opt}(\boldsymbol{u}, \Gamma) = \int_\Omega \psi_\varepsilon(\boldsymbol{\varepsilon})\mathrm{d}\Omega + \int_\Gamma G_c \mathrm{d}S - \int_\Omega \boldsymbol{b}\cdot\boldsymbol{u}\mathrm{d}\Omega - \int_{\partial\Omega_{h_i}} \boldsymbol{f}\cdot\boldsymbol{u}\mathrm{d}S \tag{1}$$

with the linear strain tensor $\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}(\boldsymbol{u})$ given by

$$\varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) \tag{2}$$

Isotropic linear elasticity is assumed and the elastic energy density $\psi_\varepsilon(\boldsymbol{\varepsilon})$ is given by Miehe et al. [22]

$$\psi_\varepsilon(\boldsymbol{\varepsilon}) = \frac{1}{2}\lambda\varepsilon_{ii}\varepsilon_{jj} + \mu\varepsilon_{ij}\varepsilon_{ij} \tag{3}$$

where λ and μ are Lamé constants.

In addition, the variational approach [47] states that initiation, propagation and branching of the crack $\Gamma(\boldsymbol{x}, t)$ at the time $t \in (0, T)$ for a