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A line search assisted monolithic approach for phase-field computing of brittle fracture

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Abstract

Phase-field modeling of fracture phenomena in solids is a very promising approach which has gained popularity within the last decade. However, within the finite element framework, already a two-dimensional quasi-static phase-field formulation is computationally quite demanding, mainly for the following reasons: (i) the need to resolve the small length scale inherent to the diffusive crack approximation calls for extremely fine meshes, at least locally in the crack phase-field transition zone, (ii) due to non-convexity of the related free-energy functional, a robust, but slowly converging *staggered* solution scheme based on algorithmic decoupling is typically used. In this contribution we tackle problem (ii) and propose a faster and equally accurate approach for quasi-static phase-field computing of (brittle) fracture using a *monolithic* solution scheme which is accompanied by a novel *line search* procedure to overcome the iterative convergence issues of non-convex minimization. We present a detailed critical evaluation of the approach and its comparison with the staggered scheme in terms of computational cost, accuracy and robustness.

Keywords: Phase-field; Fracture; Staggered; Monolithic; Line search

1. Introduction

The phase-field formulation of quasi-static brittle fracture is a non-linear problem with a strong coupling between the displacement field $\boldsymbol{u}$ and the crack phase-field d to be solved for. At every given loading step, it stems from the minimization problem of a free-energy functional which is typically non-convex in $(\boldsymbol{u}, d)$. A widely adopted form of this functional reads

$$\mathcal{E}(\boldsymbol{u}, d) = \int_\Omega \left[(1-d)^2\, \Psi_0^+(\boldsymbol{\varepsilon}(\boldsymbol{u})) + \Psi_0^-(\boldsymbol{\varepsilon}(\boldsymbol{u}))\right] \mathrm{d}\mathbf{x} + G_c \int_\Omega \left(\frac{1}{2\ell} d^2 + \frac{\ell}{2} |\nabla d|^2\right) \mathrm{d}\mathbf{x}, \tag{1}$$

see e.g. the review paper [1]. In (1), the limiting values of d, namely, $d = 0$ and $d = 1$ represent the undamaged and fully broken material phases, respectively, Ψ_0^+ and Ψ_0^- are the so-called 'tensile' and 'compressive' parts of an additive decomposition of the elastic energy density function $\Psi_0 := \frac{1}{2}\boldsymbol{\varepsilon} : \mathbb{C} : \boldsymbol{\varepsilon} = \frac{1}{2}\lambda \mathrm{tr}^2(\boldsymbol{\varepsilon}) + \mu \mathrm{tr}(\boldsymbol{\varepsilon}^2)$, where, in turn, $\boldsymbol{\varepsilon}$ is

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the second-order infinitesimal strain tensor, $\mathbb{C}$ is the fourth-order elasticity tensor, and λ and μ are the Lamé constants. The decomposition of Ψ_0 is required in order to distinguish between fracture behavior in tension and compression, more precisely, to avoid crack growth and crack faces interpenetration in compression, and its various options are available in the literature, see [1] for an overview and [2–4] for the original ones. Finally, in (1), $0 < \ell \ll 1$ is the parameter that controls the width of the transition zone of d between the two states and G_c is the material fracture toughness.

In this contribution, we are concerned with devising an efficient computational scheme for solving the weak formulation for (1). As a starting point, we address the two possible options.

The first one is based on the idea of decoupling the weak formulation into the system of two equations which is then solved in a staggered manner: with one variable being frozen, one solves for the second one, which, in turn, is to be frozen to find an update for the first one, etc. The approach is therefore called *staggered*. The staggered solution scheme is the most commonly used, see [1–4], due to its robustness: the energy functional $\mathcal{E}$ in (1) is convex with respect to each of its arguments $\boldsymbol{u}$ and d separately. The phase-field formulation in [5–8] stemming from the Francfort and Marigo variational approach to fracture [9] and using an energy functional slightly different from (1) is solved with the alternate minimization procedure and backtracking algorithm, which is closely related to the staggered scheme. In [10], this formulation is computed with the staggered approach directly. The higher-order phase-field formulation from [11] is also solved in a staggered manner. Unfortunately, in related publications the question of efficiency of the staggered scheme is not explicitly addressed. We will show that the scheme may perform quite inefficiently: at a fixed loading step a significant amount of staggered iterations is typically required to achieve energy convergence, thus resulting in a high computational cost.

In this context, the alternative scheme implying the solution of the weak formulation for (1) for both variables simultaneously (more precisely, their increments) seems more promising. Such approach is called *monolithic*. Provided that iterative convergence is achieved, the monolithic solution scheme can be shown to be faster than the staggered one. However, due to non-convexity of the functional $\mathcal{E}$ in (1) with respect to $(\boldsymbol{u}, d)$, the Newton–Raphson iterative process typically diverges, particularly in case of the so-called brutal crack evolution and in the post-peak regime of loading. To the best of our knowledge, only a few results related to some extent to the fully monolithic treatment of the problem at hand have been published so far, namely, [12] and [13]. In [12], the weak equation is augmented according to a dissipation-based arc-length procedure [14] and the resulting system is computed monolithically. Unfortunately, no discussion is provided on iterative convergence issues associated with the non-convexity of $\mathcal{E}$ in this case. In [13], the latter issues are acknowledged and tackled through a 'convexification' trick, which implies the replacement of the unknown d in the elastic part of the derivative $\mathcal{E}'$ by a fixed known extrapolation $\tilde{d}$ and application of the monolithic scheme to the already modified equation. As mentioned by the authors, 'this treatment is shown in subsequent examples to be numerically robust', yet 'the theoretical validity of the extrapolation remains an open question'.

In this contribution, we develop a procedure to restore iterative convergence of the fully monolithic scheme. This is achieved by implanting a new version of the so-called *line search* into the Newton–Raphson method. In the mechanics literature, this combination is sometimes called 'damped Newton–Raphson method' and is typically used in non-linear problems to facilitate and speed up convergence of the standard Newton–Raphson procedure, or of its variants (modified Newton's method, quasi-Newton method, etc.), see e.g. [15–19]. In phase-field computing of fracture, we propose to activate our line search procedure when divergence of the Newton–Raphson iterative scheme is detected. We, moreover, allow for a negative search direction, which is not done in the standard procedure, yet will be argued to be necessary and feasible herein. The resulting approach is termed 'line search assisted monolithic scheme'. It will be shown that the proposed line search overcomes iterative convergence issues and saves a significant amount of computational time in comparison with the staggered approach.

The paper is structured as follows. Section 2 introduces explicitly the weak formulation stemming from the minimization problem for $\mathcal{E}$ in (1) equipped with the appropriate irreversibility condition for the fracture phase-field, as well as the benchmark problem chosen for testing the existing and newly proposed solution approaches. Section 3 is devoted to the staggered scheme and to the detailed evaluation of its efficiency. In Section 4, we first address the original monolithic scheme and illustrate the related convergence issues which appear already at early stages of the modeled crack propagation. Our line search procedure is then presented and a critical comparison of the results obtained with the two approaches follows. Conclusions and outlook finalize the paper.

Throughout the paper we use the abbreviations STAG, MON and MON-ls to denote, respectively, the staggered, the monolithic and the line search assisted monolithic approaches.

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