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A convergence study of phase-field models for brittle fracture

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ABSTRACT

A crucial issue in phase-field models for brittle fracture is whether the functional that describes the distributed crack converges to the functional of the discrete crack when the internal length scale introduced in the distribution function goes to zero. Theoretical proofs exist for the original theory. However, for continuous media as well as for discretised media, significant errors have been reported in numerical solutions regarding the approximated crack surface, and hence for the dissipated energy. We show that for a practical setting, where the internal length scale and the spacing of the discretisation are small but finite, the observed discrepancy partially stems from the fact that numerical studies consider specimens of a finite length, and partially relates to the irreversibility introduced when casting the variational theory for brittle fracture in a damage-like format. While some form of irreversibility may be required in numerical implementations, the precise form significantly influences the accuracy and convergence towards the discrete crack.

1. Introduction

Discrete models, in which the original geometry is modified during the computation to account for the propagation of a discontinuity are intuitive, and improvements such as remeshing [35,12,31] and extended finite element methods [3,26,36,7] have provided ways to decouple the path of a propagating discontinuity from the original discretisation. Still, issues remain, such as the proper modelling of curved interfaces in three dimensions, and the robust implementation in three dimensions, which is a non-trivial task, neither when using remeshing, nor when exploiting the partition of unity concept as in extended finite elements. These drawbacks have promulgated the development and use of distributed, or smeared approaches, where the discontinuity is distributed over a finite width.

In this context, phase-field models have become increasingly popular for simulating a host of physical phenomena which exhibit sharp interfaces. Examples are the modelling of solidification processes, spinodal decomposition, coarsening of precipitate phases, shape memory effects, re-crystallisation, and dislocation dynamics, see e.g., [14,15,25,32,20] for overviews. The central idea behind phase-field models is that a discontinuous interface – where a Heaviside function placed at the interface models the jump in the primary variable – is replaced by a smooth function with a steep slope locally. This implies that in the gradients of the primary variable, the Dirac delta function is replaced by a regularised Dirac function, Fig. 1.

The application of phase-field models to fracture is particularly interesting and challenging. Pioneering work has been done by Francfort and Marigo [16] and Bourdin et al. [11], who proposed a phase-field approximation of the variational formulation for Griffith's theory of brittle fracture based on the Mumford-Shah potential [27]. A numerical implementation

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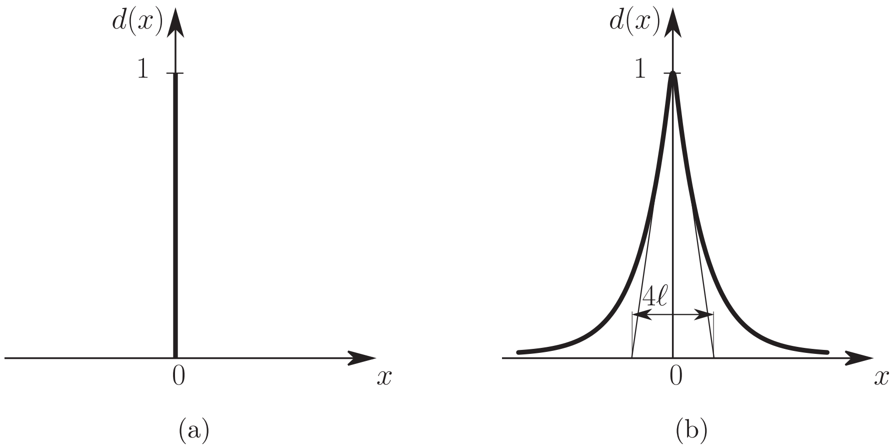

Fig. 1. (a) A sharp discontinuity, and (b) distributed discontinuity, smeared using the length scale parameter ℓ.

and examples were provided in Bourdin et al. [10] and Bourdin [9]. In this so-called variational approach to brittle fracture a sharp crack is distributed over a small, but finite width, that is proportional to an internal length scale ℓ, Fig. 1. Accordingly, the fracture energy, i.e. the energy that is needed to create a unit area of fully developed crack, is distributed over a finite zone. In this variational approach to brittle fracture, gradients are included in the functional, similar to gradient-enhanced damage models [6,17,28]. The point of departure of both models, however, is different. In gradient damage models a mechanical approach is followed, and the damage model is regularised by adding gradients to restore well-posedness of the boundary value problem in the post-peak regime. The basic idea of phase-field models, on the other hand, is to replace the zero-width discontinuity by a small, but finite zone with sharp spatial gradients in a mathematically consistent manner.

More recently, Miehe and co-workers [23,24] have exploited the similarities between phase-field theories for brittle fracture and gradient-enhanced damage models to cast phase-field models for brittle fracture in a damage format by explicitly utilising notions like a degradation function, and a damage loading function to set the irreversibility of damage. Indeed, the phase-field variable was interpreted in a manner that is synonymous to the damage variable in scalar-based damage models, starting at zero for a virgin material, and monotonically increasing to one when the material has lost all coherence. Recently, it has been shown that this formulation of the phase-field model for brittle fracture can be made identical to gradient-based damage models for a particular choice of the damage degradation function, the diffusion equation that governs the spread of the damage, and the material functions [8]. Phase-field models have now been applied to a variety of fracture problems, including dynamic fracture [5,19], cohesive fracture [33], and finite deformations [18].

A crucial issue in the phase-field approach to brittle fracture is the requirement that the functional Π_ℓ, which describes the distributed crack surface, approaches the functional Π for the discrete crack for $\ell \to 0$. When $\Pi_\ell \to \Pi$ for $\ell \to 0$, the size Γ_ℓ of the smeared crack converges to the size Γ of the discrete crack. For a continuous medium such a proof exists [13], and in Bellettini and Coscia [2] this proof has been given for a discrete medium, i.e. $\Pi_{\ell,h}$ converges to Π for $\ell \to 0$ under the condition that $h \ll \ell$, where h is the mesh spacing. Doubt has been cast on whether Γ-convergence can be achieved in actual computations, since, using the phase-field model for brittle fracture as developed by Miehe et al. [23,24], Vignollet et al. [34] and May et al. [22] have shown by numerical analyses of some simple boundary value problems that there exists a ratio ℓ/h for which the difference $|\Gamma_\ell - \Gamma|$ attains a minimum. Moreover, at this minimum the error can amount to values of 15–20%, suggesting a significant error even for the optimal discretisation.

Herein, we will show that this discrepancy is related to boundary effects, i.e. the effect of a specimen of a finite size, and to the introduction of a history variable that enforces irreversibility of the damage evolution. The convergence proofs [13,2] are for the original variational formulation of Griffith's theory [16], including its regularised form [10], where the phase-field parameter merely serves as an order parameter, and is not given the role of a history variable as in Miehe et al. [23,24].

To provide a proper setting we start by giving a brief outline of the phase-field representation of a discontinuity, and the phase-field model for brittle fracture. This is followed by an in-depth numerical analysis of a simple, but illustrative one-dimensional problem, which provides detailed information and serves to fully explain the observed discrepancy. Concluding remarks complete the paper.

2. The phase-field approach to brittle fracture

2.1. Phase-field representation of a discontinuity

The basic idea of phase-field models is to approximate a discontinuity Γ by a smeared surface Γ_ℓ. In a one-dimensional setting the exponential function