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Isogeometric analysis and hierarchical refinement for higher-order phase-field models

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Highlights

- We present a hierarchical refinement scheme for isogeometric analysis.
- We investigate different higher-order phase-field models.
- A Kuramoto–Sivashinsky system.
- A higher order phase-field approach to 3D brittle fracture.
- A higher order temperature controlled diffusion in polymer blends.

Abstract

While the interest in higher-order models in physics and mechanics grows, their numerical simulation still poses a challenge, especially for arbitrary shaped three-dimensional domains. This contribution presents the mathematical framework as well as the application to different problems in the field of material science, fracture mechanics and diffusion problems. All models under consideration require at least C^1 continuity, which prevents the application of standard finite element analysis and local mesh refinements.

Introducing isogeometric analysis (IGA) for the discretization in a finite element framework enables us to deal with these requirements. Moreover, a general hierarchical refinement scheme based on a subdivision projection is presented here for one, two and three dimensional simulations. This technique allows to enhance the approximation space using finer splines on each level but preserves the partition of unity as well as the continuity properties of the original discretization.

Using this mathematical framework, the improved convergence of a Kuramoto–Sivashinsky model, a mesh-adapted thermal diffusion simulation and computations of a priori unknown crack propagation in different fracture modes underline the versatility of the presented hierarchical refinement scheme.

Keywords: Thermal diffusion; Fracture; Phase field; Hierarchical refinement; NURBS

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1. Introduction

Phase-field models have gained raising attention for numerical simulations of a broad range of physical phenomena throughout the past years. In combination with finite element based solution strategies they enable a fascinating variety of multi-field and multi-physics simulations, cf. [1–5] and many others. In order to demonstrate the capabilities of the presented mathematical framework an in-depth investigation of a series of higher-order problems is presented.

We start with a Kuramoto–Sivashinsky system, cf. [6,7,3]. The Kuramoto–Sivashinsky model has been derived for the simulation of different thermodynamical systems far away from equilibrium state, e.g., fluctuations in fluid films and instabilities in laminar flame fronts, see, Paniconi and Elder [3], among many others. This transient fourth-order evolution equation accounts for the physics of arising chaotic instabilities in the spatial as well as the temporal domain and allows us to investigate the consistency as well as the convergence of local refinement schemes in one and two dimensions. The numerical solution of the fourth-order operator is traditionally realized using finite difference schemes. In the context of FEA for irreducible systems, global C^1 continuity is required, see Gomez and Paris [6] for the application of NURBS basis functions.

To demonstrate the capabilities in three dimensions we study a higher-order phase-field approach to brittle fracture within a fully non-linear framework along with a structure-preserving time integration, cf. [8,9]. Classical brittle fracture mechanics of Griffith and Irwin [10,11] states that material fails locally upon the attainment of a specific fracture energy. Based on this theory phase-field methods provide a modern tool to numerically predict a priori unknown crack paths. This specific methodology relies on a variationally consistent formulation of an augmented multi-field energy functional, taking the fracture energy within an additional field equation into account. The approach has proven to be accurate and robust in two and three dimensions, see Miehe et al. [12] among many others.

Here, we propose a novel framework for general non-linear hyperelastic material models combined with a fourth-order phase-field model along with the hierarchical refinement scheme presented above. The approach for finite elasticity relies on a multiplicative decomposition of the local deformation field into a compressive and a tensile part, as proposed in Hesch and Weinberg [13], i.e., we assume that local stress induces fracturing only for tension, once a certain critical energy has been reached. The applied fourth-order model for the phase-field has been proposed in Borden et al. [8] to improve accuracy and convergence using the superior regularity of a higher-order phase-field.

Eventually, a two and three dimensional model of temperature controlled diffusion in a polymer blend is investigated, cf. [14]. In consequence of different chemical potentials of both substances diffusion will be triggered and the blend starts to decompose into two different phases. Here the order parameter of the phase field marks the mass concentration c in the domain, with $0 \leq c \leq 1$. In analogy to the previously presented phase-field model of brittle fracture, the interface between coexisting phases is a transition region of small but finite length where the order parameter changes rapidly but smoothly.

For the numerical calculations, we aim at a consistent discretization of the underlying partial differential equations in contrast to mixed approaches, which are computational inefficient due to the arising large number of unknowns. Here, we apply an isogeometric analysis (IGA) approach, which employs Non-Uniform rational B-Splines (NURBS) as finite element basis functions. NURBS basis functions allow to predefine the basis functions' continuity within their construction, see Cottrell et al. [15] for a comprehensive review. The underlying splines have local support but are not restricted to a single finite element; in the multivariate case they have a tensor product structure. These specific properties, however, turn into a major drawback for the construction of local refinement procedures which are necessary for large-scale, three-dimensional systems with locally sharp gradients or other local areas of interest.

To solve these mesh-subdivision problems T-splines have been introduced in the IGA to break the tensor product structure of the spline base, see Bazilevs et al. [16]. Because additional knots are inserted into the structure, the arising T-junctions can be considered as the IGA version of hanging nodes of standard FEA. As shown in Scott et al. [17] such refinement algorithms improve the quality of approximation but become very complex in three-dimensional domains. Additionally, restriction on the polynomial degree, on the linear dependence of T-spline blending functions and on the locality of the refinement are known.

An alternative to the element-based mesh-subdivision procedures provides the hierarchical superposition of shape functions. Such refinement methods are long known from high-order FEA, see, e.g. the work of Szabò and Babuška [18], and for B-splines they have already been introduced by Forsey and Bartels [19]. Recently, such refinements have been applied within the framework of IGA, see, e.g. Vuong et al. [20], Evans et al. [21] and Scott et al. [22]. The basic idea behind a hierarchical refinement is simple: B-spline and NURBS basis functions are replaced